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# Crystal structure of 3-(2-nitrophenyl)-1-(1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one

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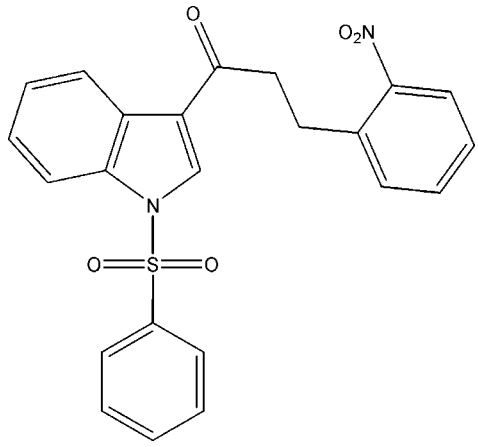
In the title compound, $C_{23}H_{18}N_2O_5S$, the phenyl and benzene rings subtend dihedral angles of 78.18 (10) and 30.18 (9)°, respectively, with the indole ring system (r.m.s. deviation = 0.022 Å). The crystal structure features weak C—H···O and C—H···$\pi$ interactions, which link the molecules into a three-dimensional network.

**Keywords:** crystal structure; indole; hydrogen bonding; C—H···$\pi$ interactions.

**CCDC reference**: 1433093

## 1. Related literature

For the biological activity of indole derivatives, see: Andreev *et al.* (2015); Kolocouris *et al.* (1994). For related structures, see: Chakkaravarthi *et al.* (2007, 2008).




## 2. Experimental

### 2.1. Crystal data

$C_{23}H_{18}N_2O_5S$
$M_r$ = 434.45
Monoclinic, $P2_1/n$
$a$ = 9.0224 (7) Å
$b$ = 15.4581 (10) Å
$c$ = 15.1347 (10) Å
$\beta$ = 106.349 (2)°
$V$ = 2025.5 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 295 K
0.26 × 0.24 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.950, $T_{max}$ = 0.961
29555 measured reflections
6149 independent reflections
4060 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.144
$S$ = 1.09
6149 reflections
280 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

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

*Cg*3 is the centroid of the C7–C12 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9···O2$^{i}$ | 0.93 | 2.54 | 3.328 (2) | 143 |
| C22—H22···O3$^{ii}$ | 0.93 | 2.42 | 3.319 (3) | 163 |
| C23—H23···O5$^{iii}$ | 0.93 | 2.36 | 3.247 (3) | 160 |
| C16—H16*A*···*Cg*3$^{iv}$ | 0.97 | 2.73 | 3.565 (2) | 144 |

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

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

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7524).

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# supporting information

*Acta Cryst.* (2015). E**71**, o892–o893 [https://doi.org/10.1107/S2056989015020162]

## Crystal structure of 3-(2-nitrophenyl)-1-(1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one

**M. Umadevi, Potharaju Raju, R. Yamuna, Arasambattu K. Mohanakrishnan and G. Chakkaravarthi**

### S1. Structural commentary

Indole derivatives are known to exhibit anti-hepatitis C virus (Andreev *et al.*, 2015) and antiviral activity (Kolocouris *et al.*, 1994). We herein report the crystal structure of (I) (Fig. 1). The *ORTEP* diagram of the title compound (I) is shown in Fig. 1. The geometric parameters of (I) are comparable with similar structures (Chakkaravarthi *et al.* 2007, 2008).

The phenyl ring (C1—C6) and benzene ring (C18—C23) make the dihedral angles of 78.18 (10)° and 30.18 (9)°, respectively with the indole ring system. The phenyl (C1—C6) and benzene (C18—C23) rings are inclined at angle of 69.93 (12)°. In the crystal structure, the intermolecular weak C—H···O and C—H···$\pi$ (Fig. 2 & Table 1) interactions form a three dimensional network.

### S2. Synthesis and crystallization

To a solution of 1-(phenylsulfonyl)-1H-indole (0.5 g, 1.94 mmol) in dry DCM 3-(2-nitrophenyl)propanoyl chloride (0.62 g, 2.92 mmol) and $SnCl_4$ (0.76 g, 2.92 mmol) were added slowly at 273 K under nitrogen atmosphere and the resulting mixture was stirred at room temperature for 30 min after completion of starting material (monitored by TLC), the reaction mass was poured over ice water containing Conc. HCl (3 ml) and extracted with DCM (20 ml). The combined organic extracts were washed with water (30 ml), brine solution (10 ml) and dried $Na_2SO_4$. Removal of solvent followed by recrystallization of the crude product from methanol (3 ml) solution afforded the title compound as colourless blocks.

### S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2Ueq(C) for C—H and C—H = 0.97 Å and $U_{iso}$(H) = 1.2Ueq(C) for $CH_2$. The reflection (0 1 1) is omitted during refinement which is owing poor agreement.

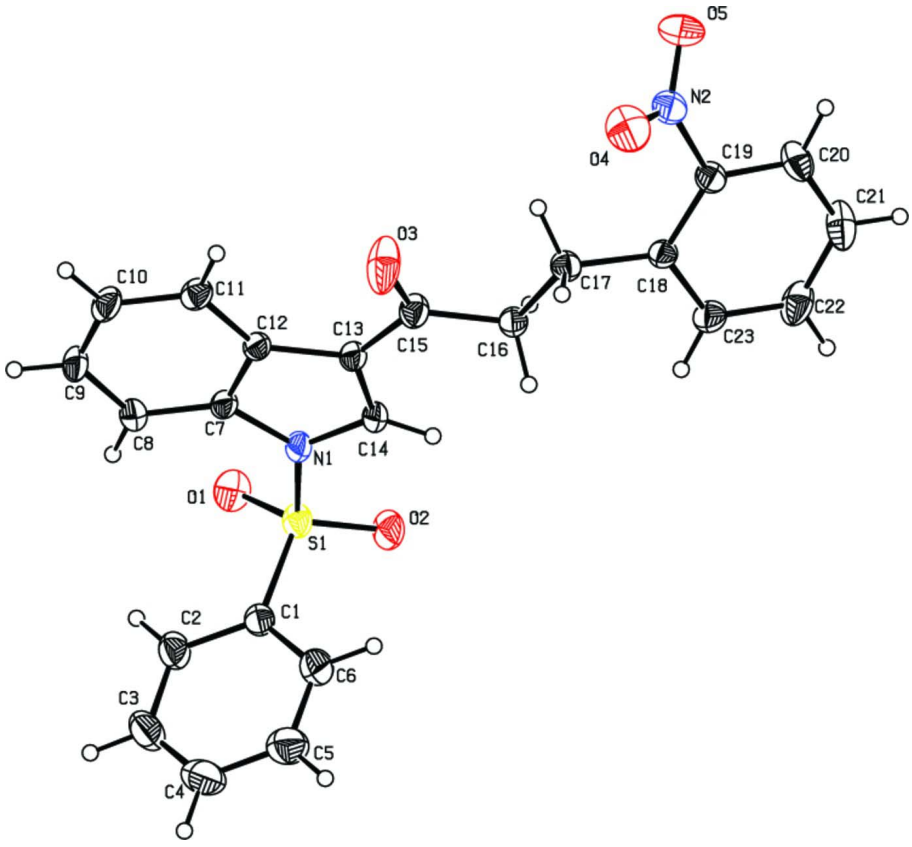


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

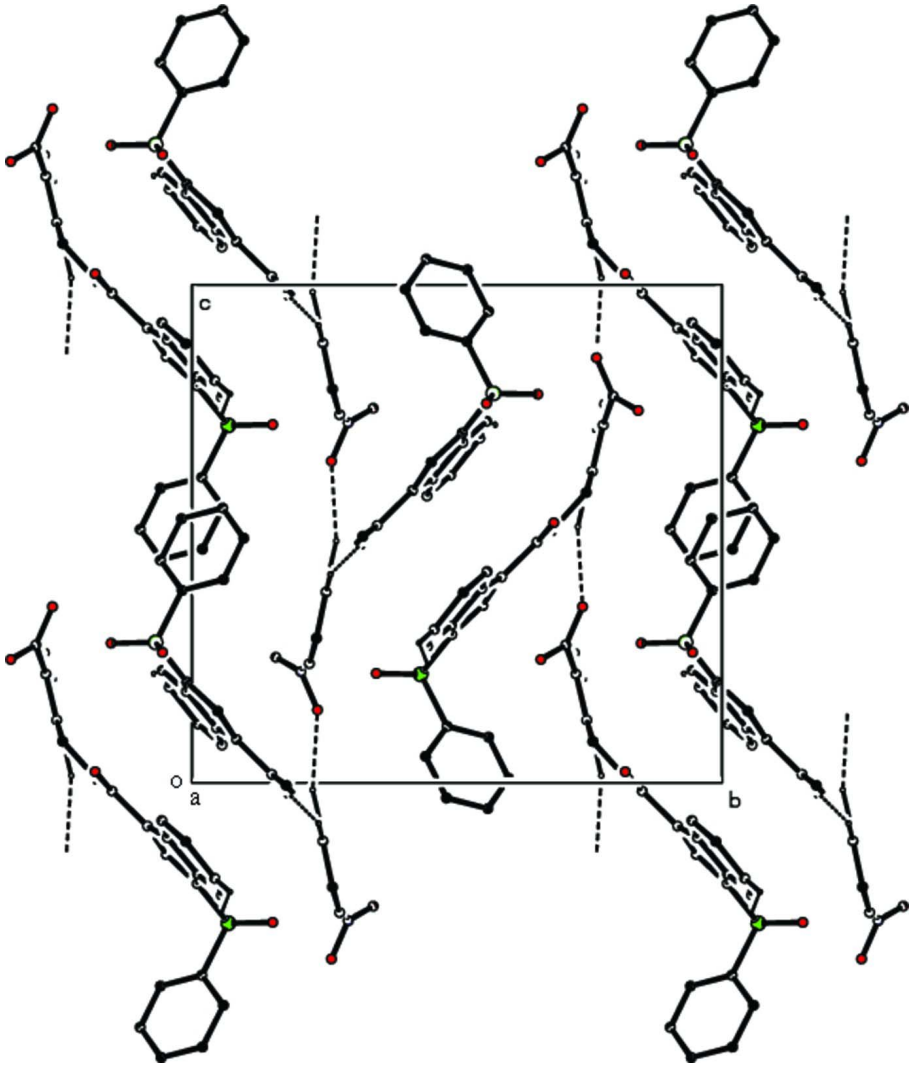


**Figure 2**

The crystal packing of the title compound, viewed along the a axis. The C—H···O hydrogen bonds are shown as dashed lines (see Table 1). H atoms not involved in these interactions have been omitted for clarity.

**3-(2-Nitrophenyl)-1-(1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one**

*Crystal data*

$C_{23}H_{18}N_2O_5S$
$M_r = 434.45$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.0224\ (7)$ Å
$b = 15.4581\ (10)$ Å
$c = 15.1347\ (10)$ Å
$\beta = 106.349\ (2)°$
$V = 2025.5\ (2)$ Å$^3$
$Z = 4$
$F(000) = 904$
$D_x = 1.425$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7714 reflections
$\theta = 2.4–28.3°$
$\mu = 0.20$ mm$^{-1}$
$T = 295$ K
Block, colourless
0.26 × 0.24 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.950, $T_{max}$ = 0.961
29555 measured reflections
6149 independent reflections
4060 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 31.6°, $\theta_{min}$ = 2.4°
$h$ = −12→11
$k$ = −21→22
$l$ = −21→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.144
$S$ = 1.09
6149 reflections
280 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 1.0896P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

*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 | 0.7579 (2) | −0.01858 (14) | 0.38658 (13) | 0.0384 (4) |
| C2 | 0.6908 (3) | −0.05928 (17) | 0.44691 (16) | 0.0514 (6) |
| H2 | 0.6403 | −0.1120 | 0.4318 | 0.062* |
| C3 | 0.7005 (3) | −0.0197 (2) | 0.53057 (17) | 0.0663 (8) |
| H3 | 0.6565 | −0.0460 | 0.5724 | 0.080* |
| C4 | 0.7746 (3) | 0.0580 (2) | 0.55179 (18) | 0.0690 (8) |
| H4 | 0.7801 | 0.0842 | 0.6079 | 0.083* |
| C5 | 0.8408 (3) | 0.09752 (19) | 0.49126 (18) | 0.0655 (7) |
| H5 | 0.8907 | 0.1504 | 0.5065 | 0.079* |
| C6 | 0.8337 (3) | 0.05935 (16) | 0.40815 (16) | 0.0527 (6) |
| H6 | 0.8793 | 0.0857 | 0.3671 | 0.063* |
| C7 | 0.4643 (2) | −0.01056 (13) | 0.18344 (12) | 0.0327 (4) |
| C8 | 0.3702 (2) | −0.05590 (14) | 0.22590 (14) | 0.0400 (5) |
| H8 | 0.4111 | −0.0932 | 0.2749 | 0.048* |
| C9 | 0.2134 (2) | −0.04298 (15) | 0.19192 (15) | 0.0445 (5) |
| H9 | 0.1467 | −0.0715 | 0.2191 | 0.053* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.1528 (2) | 0.01177 (15) | 0.11793 (15) | 0.0445 (5) |
| H10 | 0.0463 | 0.0184 | 0.0961 | 0.053* |
| C11 | 0.2462 (2) | 0.05662 (13) | 0.07591 (14) | 0.0390 (4) |
| H11 | 0.2039 | 0.0927 | 0.0260 | 0.047* |
| C12 | 0.4060 (2) | 0.04658 (12) | 0.11020 (12) | 0.0314 (4) |
| C13 | 0.5371 (2) | 0.08392 (13) | 0.08696 (13) | 0.0330 (4) |
| C14 | 0.6664 (2) | 0.04867 (13) | 0.14399 (13) | 0.0349 (4) |
| H14 | 0.7669 | 0.0618 | 0.1438 | 0.042* |
| C15 | 0.5289 (2) | 0.15065 (14) | 0.01681 (14) | 0.0407 (5) |
| C16 | 0.6745 (2) | 0.17783 (14) | −0.00516 (13) | 0.0365 (4) |
| H16A | 0.7236 | 0.1273 | −0.0225 | 0.044* |
| H16B | 0.7453 | 0.2027 | 0.0494 | 0.044* |
| C17 | 0.6424 (2) | 0.24371 (14) | −0.08307 (13) | 0.0375 (4) |
| H17A | 0.5508 | 0.2259 | −0.1306 | 0.045* |
| H17B | 0.6201 | 0.2991 | −0.0596 | 0.045* |
| C18 | 0.7729 (2) | 0.25523 (12) | −0.12581 (12) | 0.0331 (4) |
| C19 | 0.7489 (2) | 0.27562 (13) | −0.21829 (13) | 0.0375 (4) |
| C20 | 0.8658 (3) | 0.27853 (15) | −0.26069 (16) | 0.0512 (6) |
| H20 | 0.8433 | 0.2895 | −0.3235 | 0.061* |
| C21 | 1.0150 (3) | 0.26509 (17) | −0.2093 (2) | 0.0612 (7) |
| H21 | 1.0954 | 0.2681 | −0.2364 | 0.073* |
| C22 | 1.0444 (3) | 0.24708 (17) | −0.11702 (19) | 0.0583 (7) |
| H22 | 1.1457 | 0.2387 | −0.0814 | 0.070* |
| C23 | 0.9255 (2) | 0.24134 (15) | −0.07669 (15) | 0.0452 (5) |
| H23 | 0.9485 | 0.2277 | −0.0144 | 0.054* |
| N1 | 0.62637 (18) | −0.00978 (11) | 0.20252 (11) | 0.0368 (4) |
| N2 | 0.5930 (2) | 0.29460 (14) | −0.27675 (13) | 0.0504 (4) |
| O1 | 0.68799 (19) | −0.15240 (10) | 0.28042 (12) | 0.0548 (4) |
| O2 | 0.89596 (16) | −0.05570 (11) | 0.26200 (11) | 0.0528 (4) |
| O3 | 0.40514 (19) | 0.18257 (14) | −0.02227 (16) | 0.0843 (7) |
| O4 | 0.5110 (2) | 0.34181 (14) | −0.24777 (13) | 0.0738 (6) |
| O5 | 0.5554 (2) | 0.26312 (16) | −0.35371 (12) | 0.0846 (7) |
| S1 | 0.75288 (6) | −0.06854 (4) | 0.28195 (4) | 0.04012 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0297 (10) | 0.0474 (12) | 0.0366 (10) | 0.0047 (8) | 0.0069 (8) | 0.0104 (9) |
| C2 | 0.0462 (13) | 0.0614 (15) | 0.0479 (13) | −0.0007 (11) | 0.0153 (10) | 0.0164 (11) |
| C3 | 0.0641 (17) | 0.094 (2) | 0.0461 (13) | 0.0018 (16) | 0.0239 (12) | 0.0168 (14) |
| C4 | 0.0702 (18) | 0.092 (2) | 0.0437 (13) | 0.0085 (16) | 0.0135 (12) | −0.0041 (14) |
| C5 | 0.0732 (18) | 0.0651 (17) | 0.0550 (15) | −0.0096 (14) | 0.0130 (13) | −0.0070 (13) |
| C6 | 0.0536 (14) | 0.0578 (15) | 0.0476 (13) | −0.0061 (11) | 0.0155 (11) | 0.0091 (11) |
| C7 | 0.0253 (9) | 0.0404 (10) | 0.0338 (9) | −0.0015 (7) | 0.0106 (7) | −0.0059 (8) |
| C8 | 0.0353 (10) | 0.0500 (12) | 0.0379 (10) | −0.0038 (9) | 0.0153 (8) | 0.0015 (9) |
| C9 | 0.0327 (10) | 0.0569 (13) | 0.0499 (12) | −0.0094 (9) | 0.0217 (9) | −0.0047 (10) |
| C10 | 0.0249 (9) | 0.0551 (13) | 0.0551 (12) | −0.0025 (9) | 0.0137 (9) | −0.0089 (11) |
| C11 | 0.0297 (10) | 0.0428 (11) | 0.0431 (11) | 0.0032 (8) | 0.0078 (8) | −0.0022 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0278 (9) | 0.0348 (9) | 0.0327 (9) | −0.0012 (7) | 0.0104 (7) | −0.0058 (7) |
| C13 | 0.0285 (9) | 0.0379 (10) | 0.0345 (9) | −0.0014 (7) | 0.0118 (7) | −0.0030 (8) |
| C14 | 0.0262 (9) | 0.0450 (11) | 0.0356 (9) | −0.0024 (8) | 0.0121 (7) | 0.0008 (8) |
| C15 | 0.0320 (10) | 0.0450 (11) | 0.0458 (11) | 0.0016 (9) | 0.0121 (8) | 0.0065 (9) |
| C16 | 0.0304 (10) | 0.0447 (11) | 0.0333 (9) | −0.0010 (8) | 0.0071 (7) | 0.0069 (8) |
| C17 | 0.0341 (10) | 0.0439 (11) | 0.0341 (10) | 0.0030 (8) | 0.0088 (8) | 0.0061 (8) |
| C18 | 0.0316 (9) | 0.0346 (9) | 0.0312 (9) | −0.0012 (8) | 0.0057 (7) | 0.0035 (7) |
| C19 | 0.0391 (9) | 0.0370 (10) | 0.0352 (9) | 0.0011 (8) | 0.0084 (7) | 0.0092 (8) |
| C20 | 0.0593 (15) | 0.0524 (13) | 0.0483 (12) | 0.0049 (11) | 0.0258 (11) | 0.0171 (10) |
| C21 | 0.0493 (14) | 0.0625 (16) | 0.0833 (19) | 0.0094 (12) | 0.0377 (13) | 0.0260 (14) |
| C22 | 0.0299 (11) | 0.0644 (16) | 0.0780 (17) | 0.0042 (10) | 0.0108 (11) | 0.0224 (13) |
| C23 | 0.0353 (11) | 0.0550 (13) | 0.0400 (11) | −0.0012 (9) | 0.0020 (8) | 0.0097 (10) |
| N1 | 0.0247 (7) | 0.0512 (10) | 0.0353 (8) | −0.0006 (7) | 0.0096 (6) | 0.0061 (7) |
| N2 | 0.0463 (9) | 0.0630 (12) | 0.0374 (10) | 0.0006 (8) | 0.0042 (7) | 0.0201 (9) |
| O1 | 0.0543 (10) | 0.0441 (9) | 0.0673 (11) | 0.0027 (7) | 0.0192 (8) | 0.0051 (8) |
| O2 | 0.0296 (8) | 0.0740 (11) | 0.0580 (9) | 0.0098 (7) | 0.0173 (7) | 0.0095 (8) |
| O3 | 0.0350 (9) | 0.1001 (16) | 0.1185 (17) | 0.0172 (9) | 0.0228 (10) | 0.0669 (14) |
| O4 | 0.0556 (11) | 0.0885 (14) | 0.0741 (13) | 0.0308 (9) | 0.0130 (9) | 0.0299 (10) |
| O5 | 0.0781 (14) | 0.1281 (19) | 0.0350 (9) | −0.0157 (13) | −0.0045 (9) | 0.0106 (11) |
| S1 | 0.0301 (2) | 0.0473 (3) | 0.0443 (3) | 0.0062 (2) | 0.0126 (2) | 0.0080 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.378 (3) | C14—N1 | 1.383 (2) |
| C1—C2 | 1.381 (3) | C14—H14 | 0.9300 |
| C1—S1 | 1.751 (2) | C15—O3 | 1.212 (3) |
| C2—C3 | 1.387 (4) | C15—C16 | 1.502 (3) |
| C2—H2 | 0.9300 | C16—C17 | 1.523 (3) |
| C3—C4 | 1.367 (4) | C16—H16A | 0.9700 |
| C3—H3 | 0.9300 | C16—H16B | 0.9700 |
| C4—C5 | 1.370 (4) | C17—C18 | 1.505 (3) |
| C4—H4 | 0.9300 | C17—H17A | 0.9700 |
| C5—C6 | 1.374 (3) | C17—H17B | 0.9700 |
| C5—H5 | 0.9300 | C18—C23 | 1.385 (3) |
| C6—H6 | 0.9300 | C18—C19 | 1.391 (3) |
| C7—C8 | 1.391 (3) | C19—C20 | 1.381 (3) |
| C7—C12 | 1.399 (3) | C19—N2 | 1.465 (3) |
| C7—N1 | 1.408 (2) | C20—C21 | 1.368 (4) |
| C8—C9 | 1.377 (3) | C20—H20 | 0.9300 |
| C8—H8 | 0.9300 | C21—C22 | 1.375 (4) |
| C9—C10 | 1.387 (3) | C21—H21 | 0.9300 |
| C9—H9 | 0.9300 | C22—C23 | 1.379 (3) |
| C10—C11 | 1.377 (3) | C22—H22 | 0.9300 |
| C10—H10 | 0.9300 | C23—H23 | 0.9300 |
| C11—C12 | 1.397 (3) | N1—S1 | 1.6736 (17) |
| C11—H11 | 0.9300 | N2—O4 | 1.207 (3) |
| C12—C13 | 1.445 (2) | N2—O5 | 1.219 (3) |
| C13—C14 | 1.355 (3) | O1—S1 | 1.4199 (17) |

| | | | |
|---|---|---|---|
| C13—C15 | 1.467 (3) | O2—S1 | 1.4200 (15) |
| | | | |
| C6—C1—C2 | 121.5 (2) | C13—C15—C16 | 119.20 (17) |
| C6—C1—S1 | 118.98 (16) | C15—C16—C17 | 111.76 (16) |
| C2—C1—S1 | 119.51 (18) | C15—C16—H16A | 109.3 |
| C1—C2—C3 | 118.4 (2) | C17—C16—H16A | 109.3 |
| C1—C2—H2 | 120.8 | C15—C16—H16B | 109.3 |
| C3—C2—H2 | 120.8 | C17—C16—H16B | 109.3 |
| C4—C3—C2 | 120.2 (2) | H16A—C16—H16B | 107.9 |
| C4—C3—H3 | 119.9 | C18—C17—C16 | 114.23 (16) |
| C2—C3—H3 | 119.9 | C18—C17—H17A | 108.7 |
| C3—C4—C5 | 120.7 (3) | C16—C17—H17A | 108.7 |
| C3—C4—H4 | 119.6 | C18—C17—H17B | 108.7 |
| C5—C4—H4 | 119.6 | C16—C17—H17B | 108.7 |
| C4—C5—C6 | 120.2 (3) | H17A—C17—H17B | 107.6 |
| C4—C5—H5 | 119.9 | C23—C18—C19 | 115.16 (18) |
| C6—C5—H5 | 119.9 | C23—C18—C17 | 122.06 (17) |
| C5—C6—C1 | 119.0 (2) | C19—C18—C17 | 122.69 (17) |
| C5—C6—H6 | 120.5 | C20—C19—C18 | 123.49 (19) |
| C1—C6—H6 | 120.5 | C20—C19—N2 | 116.22 (18) |
| C8—C7—C12 | 122.82 (17) | C18—C19—N2 | 120.29 (18) |
| C8—C7—N1 | 130.07 (18) | C21—C20—C19 | 119.3 (2) |
| C12—C7—N1 | 107.11 (16) | C21—C20—H20 | 120.4 |
| C9—C8—C7 | 116.8 (2) | C19—C20—H20 | 120.4 |
| C9—C8—H8 | 121.6 | C20—C21—C22 | 119.1 (2) |
| C7—C8—H8 | 121.6 | C20—C21—H21 | 120.4 |
| C8—C9—C10 | 121.31 (19) | C22—C21—H21 | 120.4 |
| C8—C9—H9 | 119.3 | C21—C22—C23 | 120.7 (2) |
| C10—C9—H9 | 119.3 | C21—C22—H22 | 119.6 |
| C11—C10—C9 | 121.80 (19) | C23—C22—H22 | 119.6 |
| C11—C10—H10 | 119.1 | C22—C23—C18 | 122.2 (2) |
| C9—C10—H10 | 119.1 | C22—C23—H23 | 118.9 |
| C10—C11—C12 | 118.3 (2) | C18—C23—H23 | 118.9 |
| C10—C11—H11 | 120.8 | C14—N1—C7 | 108.51 (15) |
| C12—C11—H11 | 120.8 | C14—N1—S1 | 124.51 (13) |
| C11—C12—C7 | 118.88 (17) | C7—N1—S1 | 126.97 (13) |
| C11—C12—C13 | 134.02 (18) | O4—N2—O5 | 123.7 (2) |
| C7—C12—C13 | 107.10 (16) | O4—N2—C19 | 119.0 (2) |
| C14—C13—C12 | 107.52 (17) | O5—N2—C19 | 117.3 (2) |
| C14—C13—C15 | 127.04 (17) | O1—S1—O2 | 121.30 (10) |
| C12—C13—C15 | 125.39 (17) | O1—S1—N1 | 106.80 (9) |
| C13—C14—N1 | 109.73 (16) | O2—S1—N1 | 104.39 (9) |
| C13—C14—H14 | 125.1 | O1—S1—C1 | 108.84 (10) |
| N1—C14—H14 | 125.1 | O2—S1—C1 | 109.71 (10) |
| O3—C15—C13 | 119.40 (19) | N1—S1—C1 | 104.41 (9) |
| O3—C15—C16 | 121.40 (19) | | |
| | | | |
| C6—C1—C2—C3 | 0.3 (3) | C23—C18—C19—C20 | 2.7 (3) |

| | | | |
|---|---|---|---|
| S1—C1—C2—C3 | 178.00 (18) | C17—C18—C19—C20 | −173.8 (2) |
| C1—C2—C3—C4 | 0.2 (4) | C23—C18—C19—N2 | −177.95 (19) |
| C2—C3—C4—C5 | −0.3 (4) | C17—C18—C19—N2 | 5.6 (3) |
| C3—C4—C5—C6 | −0.1 (4) | C18—C19—C20—C21 | −3.4 (4) |
| C4—C5—C6—C1 | 0.6 (4) | N2—C19—C20—C21 | 177.3 (2) |
| C2—C1—C6—C5 | −0.7 (3) | C19—C20—C21—C22 | 1.4 (4) |
| S1—C1—C6—C5 | −178.44 (19) | C20—C21—C22—C23 | 0.9 (4) |
| C12—C7—C8—C9 | 0.6 (3) | C21—C22—C23—C18 | −1.5 (4) |
| N1—C7—C8—C9 | 179.64 (19) | C19—C18—C23—C22 | −0.2 (3) |
| C7—C8—C9—C10 | 0.9 (3) | C17—C18—C23—C22 | 176.3 (2) |
| C8—C9—C10—C11 | −1.0 (3) | C13—C14—N1—C7 | −1.3 (2) |
| C9—C10—C11—C12 | −0.6 (3) | C13—C14—N1—S1 | 178.71 (14) |
| C10—C11—C12—C7 | 2.1 (3) | C8—C7—N1—C14 | −177.3 (2) |
| C10—C11—C12—C13 | −177.6 (2) | C12—C7—N1—C14 | 1.8 (2) |
| C8—C7—C12—C11 | −2.2 (3) | C8—C7—N1—S1 | 2.6 (3) |
| N1—C7—C12—C11 | 178.61 (17) | C12—C7—N1—S1 | −178.24 (14) |
| C8—C7—C12—C13 | 177.62 (18) | C20—C19—N2—O4 | −135.8 (2) |
| N1—C7—C12—C13 | −1.6 (2) | C18—C19—N2—O4 | 44.9 (3) |
| C11—C12—C13—C14 | −179.4 (2) | C20—C19—N2—O5 | 42.3 (3) |
| C7—C12—C13—C14 | 0.8 (2) | C18—C19—N2—O5 | −137.1 (2) |
| C11—C12—C13—C15 | 3.0 (3) | C14—N1—S1—O1 | −139.88 (17) |
| C7—C12—C13—C15 | −176.77 (18) | C7—N1—S1—O1 | 40.16 (19) |
| C12—C13—C14—N1 | 0.3 (2) | C14—N1—S1—O2 | −10.27 (19) |
| C15—C13—C14—N1 | 177.84 (19) | C7—N1—S1—O2 | 169.78 (17) |
| C14—C13—C15—O3 | −172.1 (2) | C14—N1—S1—C1 | 104.91 (17) |
| C12—C13—C15—O3 | 5.0 (3) | C7—N1—S1—C1 | −75.05 (18) |
| C14—C13—C15—C16 | 8.0 (3) | C6—C1—S1—O1 | 172.14 (17) |
| C12—C13—C15—C16 | −174.90 (18) | C2—C1—S1—O1 | −5.6 (2) |
| O3—C15—C16—C17 | −3.1 (3) | C6—C1—S1—O2 | 37.3 (2) |
| C13—C15—C16—C17 | 176.79 (18) | C2—C1—S1—O2 | −140.47 (17) |
| C15—C16—C17—C18 | −164.04 (17) | C6—C1—S1—N1 | −74.09 (18) |
| C16—C17—C18—C23 | −28.2 (3) | C2—C1—S1—N1 | 108.15 (18) |
| C16—C17—C18—C19 | 148.00 (19) | | |

*Hydrogen-bond geometry (Å, º)*

Cg3 is the centroid of the C7–C12 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9···O2$^{i}$ | 0.93 | 2.54 | 3.328 (2) | 143 |
| C22—H22···O3$^{ii}$ | 0.93 | 2.42 | 3.319 (3) | 163 |
| C23—H23···O5$^{iii}$ | 0.93 | 2.36 | 3.247 (3) | 160 |
| C16—H16*A*···*Cg*3$^{iv}$ | 0.97 | 2.73 | 3.565 (2) | 144 |

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