Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (*E*)-1-[2-(4-Chloro-2-nitrostyryl)-1-phenylsulfonyl-1*H*-indol-3-yl]propan-1-one

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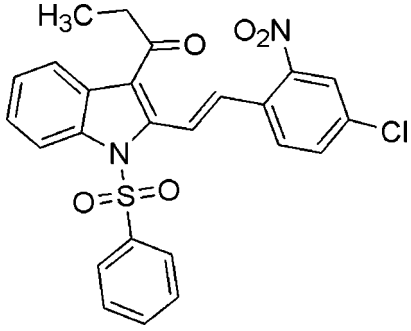
Received 8 November 2013; accepted 12 November 2013

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.050; $wR$ factor = 0.150; data-to-parameter ratio = 20.6.

In the title compound, $C_{25}H_{19}ClN_2O_5S$, the phenyl ring forms dihedral angles of 79.62 (12) and 80.02 (13)° with the indole ring system and the benzene ring, respectively. The nitro group is twisted at an angle of 22.39 (11)° with respect to the attached benzene ring. In the crystal, molecules assemble into double layers in the *ab* plane *via* C—H···O interactions.

## Related literature

For the biological activity of indole derivatives, see: Okabe & Adachi (1998); Srivastava *et al.* (2011). For related structures, see: Chakkaravarthi *et al.* (2008, 2010).




## Experimental

### Crystal data

$C_{25}H_{19}ClN_2O_5S$
$M_r$ = 494.93
Triclinic, $P\overline{1}$
$a$ = 8.4658 (3) Å
$b$ = 8.6643 (3) Å
$c$ = 16.1126 (6) Å
$\alpha$ = 84.196 (2)°
$\beta$ = 87.768 (3)°
$\gamma$ = 79.541 (2)°
$V$ = 1156.01 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.30 mm$^{-1}$
$T$ = 295 K
0.28 × 0.24 × 0.20 mm

### Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.922, $T_{max}$ = 0.943
25531 measured reflections
6333 independent reflections
4536 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.150
$S$ = 1.03
6333 reflections
308 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···O1$^{i}$ | 0.93 | 2.60 | 3.327 (3) | 136 |
| C16—H16$B$···O5$^{ii}$ | 0.97 | 2.37 | 3.260 (3) | 152 |

Symmetry codes: (i) $x, y+1, z$; (ii) $x+1, y, z$.

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*.

The authors wish to acknowledge the SAIF, IIT Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5271).

## References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chakkaravarthi, G., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2008). *Acta Cryst.* E**64**, o749.
Chakkaravarthi, G., Panchatcharam, R., Dhayalan, V., Mohanakrishnan, A. K. & Manivannan, V. (2010). *Acta Cryst.* E**66**, o2957.
Okabe, N. & Adachi, Y. (1998). *Acta Cryst.* C**54**, 386–387.
Sheldrick, G. M. (1996). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Srivastava, Anupam & Pandeya, S. N. (2011). *JCPR*, **1**, 1–17.

# supporting information

*Acta Cryst.* (2013). E**69**, o1784 [doi:10.1107/S1600536813031073]

## (*E*)-1-[2-(4-Chloro-2-nitrostyryl)-1-phenylsulfonyl-1*H*-indol-3-yl]propan-1-one

**M. Umadevi, V. Saravanan, R. Yamuna, A. K. Mohanakrishnan and G. Chakkaravarthi**

### S1. Experimental

#### S1.1. Synthesis and crystallization

A solution of 1-(2-(bromomethyl)-1-(phenylsulfonyl)-1*H*-indol-3-yl)propan-1-one (5 g, 12.31 mmol) and triphenylphosphine (3.5 g, 13.54 mmol) in dry THF (100 ml) was refluxed for 6 h. After consumption of the starting material, the solvent was removed under vacuum and the solid washed with diethyl ether to give the phosphonium salt. Then, the mixture of phosphonium salt (8 g, 11.97 mmol), 4-chloro-2-nitrobenzaldehyde (2.45 g, 13.17 mmol) and $K_2CO_3$ (3.30 g, 23.95 mmol) in DCM (70 ml) was stirred at room temperature for 24 h. After completion of the reaction (monitored by TLC), it was diluted using DCM (30 ml), washed with water (2 *x* 100 ml) and dried ($Na_2SO_4$). Removal of solvent *in vacuo* followed by trituration of the crude product with MeOH (20 ml) afforded the title compound.

#### S1.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were positioned geometrically and refined using riding model, with C—H = (0.93–0.97) Å and $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C). Owing to poor agreement, the (001) reflection was omitted from the final cycles of refinement.

### S2. Results and discussion

In continuation of our studies on indole derivatives which are known to exhibit anti-microbial, anti-biotic, analgesic and anti-cancer activities (Okabe and Adachi, 1998; Srivastava *et al.*, 2011), we herewith report the crystal structure of the title compound (I). The geometric parameters of (I) (Fig. 1) are in close agreement with similar structures (Chakkaravarthi *et al.*, 2008; 2010).

The phenyl ring makes the dihedral angle of 79.62 (12)° with the indole ring system. The phenyl ring (C1—C6) and the benzene ring (C20—C25) are inclined at an angle of 80.02 (13)°. The nitro group is twisted at an angle of 22.39 (11)° with respect to the attached benzene ring (C20—C25). The N1 atom is $sp^2$ hybridised as the bond angles around N1 atom sum 352.4°. Details of the C—H···O interactions are given in Table 2 - these lead to layers in the *ab* plane.

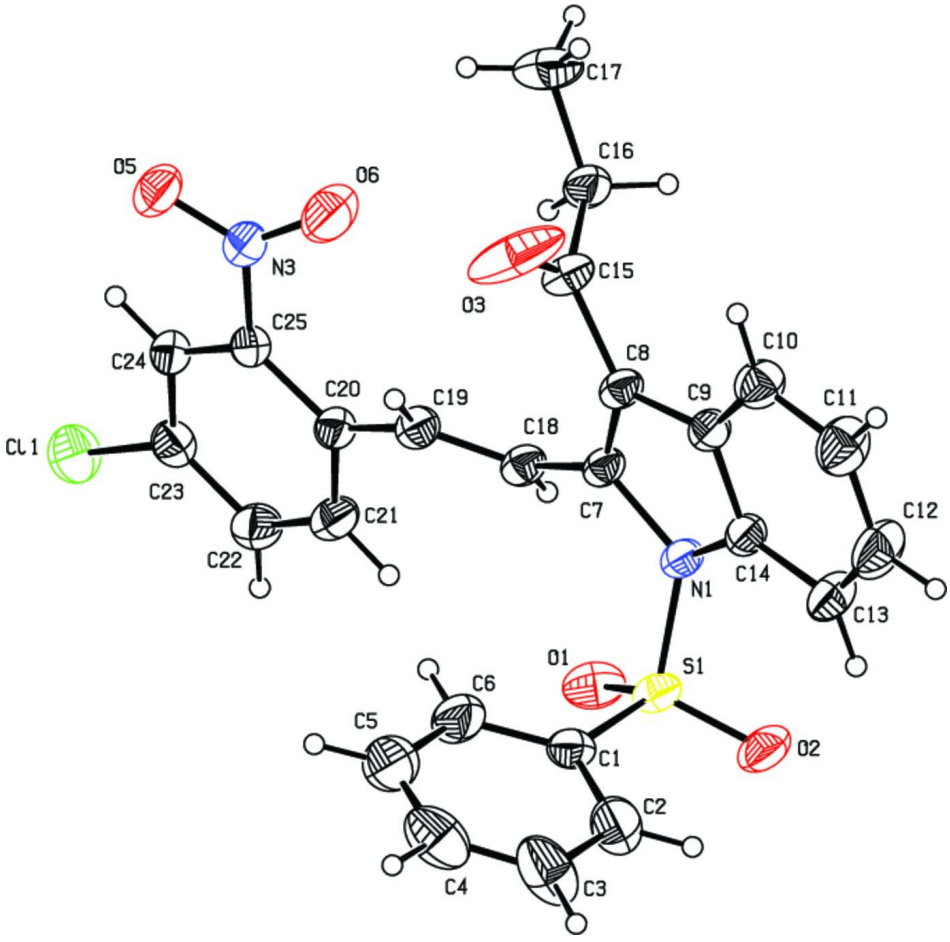



**Figure 1**

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

**(*E*)-1-[2-(4-Chloro-2-nitrostyryl)-1-phenylsulfonyl-1*H*-indol-3-yl]propan-1-one**

*Crystal data*

$C_{25}H_{19}ClN_2O_5S$
$M_r = 494.93$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.4658$ (3) Å
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$c = 16.1126$ (6) Å
$\alpha = 84.196$ (2)°
$\beta = 87.768$ (3)°
$\gamma = 79.541$ (2)°
$V = 1156.01$ (7) Å$^3$
$Z = 2$
$F(000) = 512$
$D_x = 1.422$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8917 reflections
$\theta = 2.5$–$28.4°$
$\mu = 0.30$ mm$^{-1}$
$T = 295$ K
Block, colourless
0.28 × 0.24 × 0.20 mm

*Data collection*

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.922$, $T_{max} = 0.943$
25531 measured reflections
6333 independent reflections

4536 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 29.5°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -20 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.150$
$S = 1.03$
6333 reflections
308 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
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.3517P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å$^{-3}$
$\Delta\rho_{min} = -0.39$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.6620 (2) | 0.1560 (2) | 0.44142 (11) | 0.0497 (4) |
| C2 | 0.7468 (3) | 0.1501 (4) | 0.51342 (14) | 0.0765 (7) |
| H2 | 0.8570 | 0.1131 | 0.5140 | 0.092* |
| C3 | 0.6662 (4) | 0.1997 (5) | 0.58429 (16) | 0.0984 (11) |
| H3 | 0.7215 | 0.1945 | 0.6336 | 0.118* |
| C4 | 0.5062 (4) | 0.2564 (4) | 0.58242 (17) | 0.0920 (9) |
| H4 | 0.4537 | 0.2952 | 0.6298 | 0.110* |
| C5 | 0.4199 (4) | 0.2573 (4) | 0.51124 (19) | 0.0991 (10) |
| H5 | 0.3093 | 0.2923 | 0.5115 | 0.119* |
| C6 | 0.4985 (3) | 0.2060 (3) | 0.43989 (15) | 0.0781 (7) |
| H6 | 0.4420 | 0.2053 | 0.3916 | 0.094* |
| C7 | 0.6425 (2) | 0.3393 (2) | 0.23941 (10) | 0.0408 (4) |
| C8 | 0.6569 (2) | 0.4934 (2) | 0.22907 (10) | 0.0424 (4) |
| C9 | 0.7938 (2) | 0.5131 (2) | 0.27424 (11) | 0.0439 (4) |
| C10 | 0.8617 (3) | 0.6446 (2) | 0.28430 (14) | 0.0584 (5) |
| H10 | 0.8179 | 0.7435 | 0.2589 | 0.070* |
| C11 | 0.9950 (3) | 0.6244 (3) | 0.33266 (18) | 0.0738 (7) |
| H11 | 1.0405 | 0.7113 | 0.3412 | 0.089* |
| C12 | 1.0626 (3) | 0.4773 (3) | 0.36883 (18) | 0.0771 (7) |
| H12 | 1.1536 | 0.4675 | 0.4008 | 0.093* |
| C13 | 0.9999 (3) | 0.3449 (3) | 0.35916 (15) | 0.0625 (5) |
| H13 | 1.0466 | 0.2461 | 0.3836 | 0.075* |
| C14 | 0.8635 (2) | 0.3653 (2) | 0.31128 (11) | 0.0440 (4) |
| C15 | 0.5596 (2) | 0.6261 (2) | 0.17657 (12) | 0.0516 (5) |
| C16 | 0.5615 (3) | 0.6198 (3) | 0.08490 (12) | 0.0593 (5) |
| H16A | 0.5066 | 0.5359 | 0.0729 | 0.071* |
| H16B | 0.6722 | 0.5927 | 0.0657 | 0.071* |
| C17 | 0.4848 (4) | 0.7702 (3) | 0.03593 (16) | 0.0880 (8) |
| H17A | 0.3710 | 0.7884 | 0.0469 | 0.132* |
| H17B | 0.5053 | 0.7613 | −0.0226 | 0.132* |
| H17C | 0.5291 | 0.8566 | 0.0523 | 0.132* |

| | | | | |
|---|---|---|---|---|
| C18 | 0.5229 (2) | 0.2611 (2) | 0.20724 (10) | 0.0442 (4) |
| H18 | 0.5563 | 0.1621 | 0.1884 | 0.053* |
| C19 | 0.3680 (2) | 0.3249 (2) | 0.20359 (11) | 0.0467 (4) |
| H19 | 0.3352 | 0.4250 | 0.2212 | 0.056* |
| C20 | 0.2462 (2) | 0.2449 (2) | 0.17303 (11) | 0.0453 (4) |
| C21 | 0.2582 (3) | 0.0828 (2) | 0.19095 (14) | 0.0566 (5) |
| H21 | 0.3466 | 0.0271 | 0.2201 | 0.068* |
| C22 | 0.1449 (3) | 0.0018 (2) | 0.16730 (14) | 0.0589 (5) |
| H22 | 0.1580 | −0.1070 | 0.1796 | 0.071* |
| C23 | 0.0107 (2) | 0.0832 (2) | 0.12499 (12) | 0.0518 (4) |
| C24 | −0.0071 (2) | 0.2427 (2) | 0.10536 (12) | 0.0487 (4) |
| H23 | −0.0963 | 0.2976 | 0.0764 | 0.058* |
| C25 | 0.1097 (2) | 0.3207 (2) | 0.12932 (11) | 0.0452 (4) |
| N1 | 0.77198 (17) | 0.25460 (17) | 0.28902 (9) | 0.0427 (3) |
| N3 | 0.0859 (2) | 0.4903 (2) | 0.10290 (11) | 0.0554 (4) |
| O1 | 0.6646 (2) | 0.00599 (16) | 0.31000 (9) | 0.0651 (4) |
| O2 | 0.92318 (19) | 0.02047 (18) | 0.37066 (10) | 0.0682 (4) |
| O3 | 0.4897 (3) | 0.7364 (2) | 0.20882 (12) | 0.1283 (11) |
| O5 | −0.04694 (18) | 0.55877 (18) | 0.08461 (11) | 0.0692 (4) |
| O6 | 0.2012 (2) | 0.5539 (2) | 0.09605 (17) | 0.1115 (9) |
| S1 | 0.76175 (6) | 0.08992 (5) | 0.35118 (3) | 0.04869 (14) |
| Cl1 | −0.13374 (7) | −0.01698 (7) | 0.09611 (4) | 0.07319 (19) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0570 (11) | 0.0502 (10) | 0.0409 (9) | −0.0105 (8) | −0.0042 (8) | 0.0040 (7) |
| C2 | 0.0641 (14) | 0.121 (2) | 0.0511 (12) | −0.0321 (14) | −0.0066 (10) | −0.0076 (13) |
| C3 | 0.098 (2) | 0.169 (3) | 0.0489 (13) | −0.071 (2) | 0.0058 (13) | −0.0239 (17) |
| C4 | 0.114 (3) | 0.112 (2) | 0.0570 (15) | −0.0362 (19) | 0.0260 (16) | −0.0210 (15) |
| C5 | 0.0807 (18) | 0.127 (3) | 0.0700 (17) | 0.0174 (18) | 0.0207 (14) | 0.0128 (17) |
| C6 | 0.0669 (14) | 0.106 (2) | 0.0486 (12) | 0.0085 (14) | −0.0037 (10) | 0.0089 (12) |
| C7 | 0.0405 (8) | 0.0465 (9) | 0.0314 (7) | 0.0034 (7) | −0.0039 (6) | −0.0038 (6) |
| C8 | 0.0444 (9) | 0.0458 (9) | 0.0330 (8) | 0.0039 (7) | −0.0042 (7) | −0.0044 (7) |
| C9 | 0.0421 (9) | 0.0493 (9) | 0.0373 (8) | −0.0004 (7) | −0.0008 (7) | −0.0048 (7) |
| C10 | 0.0591 (12) | 0.0499 (11) | 0.0654 (13) | −0.0074 (9) | −0.0074 (10) | −0.0043 (9) |
| C11 | 0.0639 (14) | 0.0660 (14) | 0.0959 (18) | −0.0182 (11) | −0.0190 (13) | −0.0110 (13) |
| C12 | 0.0568 (13) | 0.0819 (17) | 0.0943 (19) | −0.0116 (12) | −0.0320 (13) | −0.0059 (14) |
| C13 | 0.0503 (11) | 0.0655 (13) | 0.0677 (13) | 0.0003 (9) | −0.0196 (10) | 0.0001 (10) |
| C14 | 0.0398 (8) | 0.0495 (9) | 0.0400 (9) | −0.0013 (7) | −0.0029 (7) | −0.0035 (7) |
| C15 | 0.0597 (11) | 0.0460 (10) | 0.0443 (10) | 0.0046 (8) | −0.0140 (8) | −0.0024 (8) |
| C16 | 0.0538 (11) | 0.0768 (14) | 0.0393 (9) | 0.0031 (10) | −0.0010 (8) | 0.0057 (9) |
| C17 | 0.117 (2) | 0.0850 (18) | 0.0532 (13) | −0.0059 (16) | −0.0168 (14) | 0.0213 (12) |
| C18 | 0.0476 (9) | 0.0459 (9) | 0.0369 (8) | −0.0009 (7) | −0.0060 (7) | −0.0045 (7) |
| C19 | 0.0471 (9) | 0.0481 (10) | 0.0424 (9) | −0.0022 (8) | −0.0022 (7) | −0.0042 (7) |
| C20 | 0.0412 (9) | 0.0489 (10) | 0.0430 (9) | −0.0024 (7) | 0.0006 (7) | −0.0014 (7) |
| C21 | 0.0533 (11) | 0.0505 (11) | 0.0612 (12) | −0.0003 (9) | −0.0098 (9) | 0.0045 (9) |
| C22 | 0.0625 (12) | 0.0478 (10) | 0.0644 (13) | −0.0080 (9) | −0.0033 (10) | 0.0017 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.0503 (10) | 0.0574 (11) | 0.0486 (10) | −0.0131 (9) | 0.0045 (8) | −0.0052 (8) |
| C24 | 0.0388 (9) | 0.0563 (11) | 0.0482 (10) | −0.0044 (8) | 0.0006 (7) | −0.0001 (8) |
| C25 | 0.0395 (9) | 0.0479 (9) | 0.0447 (9) | −0.0028 (7) | 0.0035 (7) | 0.0015 (7) |
| N1 | 0.0420 (7) | 0.0436 (8) | 0.0389 (7) | 0.0004 (6) | −0.0064 (6) | 0.0001 (6) |
| N3 | 0.0441 (8) | 0.0534 (9) | 0.0655 (10) | −0.0064 (7) | −0.0053 (7) | 0.0068 (8) |
| O1 | 0.0916 (11) | 0.0455 (7) | 0.0589 (9) | −0.0115 (7) | −0.0143 (8) | −0.0052 (6) |
| O2 | 0.0624 (9) | 0.0575 (8) | 0.0722 (10) | 0.0174 (7) | −0.0096 (7) | 0.0063 (7) |
| O3 | 0.205 (3) | 0.0840 (13) | 0.0636 (11) | 0.0794 (16) | −0.0502 (14) | −0.0264 (10) |
| O5 | 0.0509 (8) | 0.0593 (9) | 0.0903 (12) | 0.0050 (7) | −0.0109 (8) | 0.0038 (8) |
| O6 | 0.0654 (11) | 0.0756 (12) | 0.189 (2) | −0.0286 (9) | −0.0420 (13) | 0.0514 (14) |
| S1 | 0.0554 (3) | 0.0407 (2) | 0.0451 (2) | 0.00326 (19) | −0.00822 (19) | 0.00039 (18) |
| Cl1 | 0.0676 (4) | 0.0741 (4) | 0.0840 (4) | −0.0276 (3) | −0.0047 (3) | −0.0088 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.374 (3) | C15—O3 | 1.185 (2) |
| C1—C2 | 1.380 (3) | C15—C16 | 1.483 (3) |
| C1—S1 | 1.747 (2) | C16—C17 | 1.506 (3) |
| C2—C3 | 1.373 (4) | C16—H16A | 0.9700 |
| C2—H2 | 0.9300 | C16—H16B | 0.9700 |
| C3—C4 | 1.355 (5) | C17—H17A | 0.9600 |
| C3—H3 | 0.9300 | C17—H17B | 0.9600 |
| C4—C5 | 1.383 (5) | C17—H17C | 0.9600 |
| C4—H4 | 0.9300 | C18—C19 | 1.329 (3) |
| C5—C6 | 1.378 (4) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—C20 | 1.468 (3) |
| C6—H6 | 0.9300 | C19—H19 | 0.9300 |
| C7—C8 | 1.355 (3) | C20—C21 | 1.391 (3) |
| C7—N1 | 1.427 (2) | C20—C25 | 1.399 (2) |
| C7—C18 | 1.454 (2) | C21—C22 | 1.373 (3) |
| C8—C9 | 1.437 (2) | C21—H21 | 0.9300 |
| C8—C15 | 1.493 (2) | C22—C23 | 1.387 (3) |
| C9—C10 | 1.393 (3) | C22—H22 | 0.9300 |
| C9—C14 | 1.394 (2) | C23—C24 | 1.369 (3) |
| C10—C11 | 1.371 (3) | C23—Cl1 | 1.725 (2) |
| C10—H10 | 0.9300 | C24—C25 | 1.382 (3) |
| C11—C12 | 1.379 (4) | C24—H23 | 0.9300 |
| C11—H11 | 0.9300 | C25—N3 | 1.468 (2) |
| C12—C13 | 1.373 (3) | N1—S1 | 1.6720 (15) |
| C12—H12 | 0.9300 | N3—O6 | 1.202 (2) |
| C13—C14 | 1.388 (3) | N3—O5 | 1.205 (2) |
| C13—H13 | 0.9300 | O1—S1 | 1.4153 (16) |
| C14—N1 | 1.418 (2) | O2—S1 | 1.4230 (15) |
| | | | |
| C6—C1—C2 | 121.4 (2) | C17—C16—H16A | 108.5 |
| C6—C1—S1 | 118.79 (16) | C15—C16—H16B | 108.5 |
| C2—C1—S1 | 119.75 (18) | C17—C16—H16B | 108.5 |
| C3—C2—C1 | 119.1 (3) | H16A—C16—H16B | 107.5 |

| | | | |
|---|---|---|---|
| C3—C2—H2 | 120.5 | C16—C17—H17A | 109.5 |
| C1—C2—H2 | 120.5 | C16—C17—H17B | 109.5 |
| C4—C3—C2 | 120.0 (3) | H17A—C17—H17B | 109.5 |
| C4—C3—H3 | 120.0 | C16—C17—H17C | 109.5 |
| C2—C3—H3 | 120.0 | H17A—C17—H17C | 109.5 |
| C3—C4—C5 | 121.1 (3) | H17B—C17—H17C | 109.5 |
| C3—C4—H4 | 119.5 | C19—C18—C7 | 122.80 (17) |
| C5—C4—H4 | 119.5 | C19—C18—H18 | 118.6 |
| C6—C5—C4 | 119.6 (3) | C7—C18—H18 | 118.6 |
| C6—C5—H5 | 120.2 | C18—C19—C20 | 123.04 (17) |
| C4—C5—H5 | 120.2 | C18—C19—H19 | 118.5 |
| C1—C6—C5 | 118.7 (2) | C20—C19—H19 | 118.5 |
| C1—C6—H6 | 120.6 | C21—C20—C25 | 115.37 (17) |
| C5—C6—H6 | 120.6 | C21—C20—C19 | 119.73 (16) |
| C8—C7—N1 | 108.46 (15) | C25—C20—C19 | 124.82 (16) |
| C8—C7—C18 | 129.63 (15) | C22—C21—C20 | 122.68 (18) |
| N1—C7—C18 | 121.90 (15) | C22—C21—H21 | 118.7 |
| C7—C8—C9 | 108.69 (15) | C20—C21—H21 | 118.7 |
| C7—C8—C15 | 128.84 (16) | C21—C22—C23 | 119.55 (19) |
| C9—C8—C15 | 122.37 (17) | C21—C22—H22 | 120.2 |
| C10—C9—C14 | 119.98 (17) | C23—C22—H22 | 120.2 |
| C10—C9—C8 | 132.32 (17) | C24—C23—C22 | 120.32 (19) |
| C14—C9—C8 | 107.70 (16) | C24—C23—Cl1 | 119.70 (16) |
| C11—C10—C9 | 118.2 (2) | C22—C23—Cl1 | 119.98 (16) |
| C11—C10—H10 | 120.9 | C23—C24—C25 | 118.76 (17) |
| C9—C10—H10 | 120.9 | C23—C24—H23 | 120.6 |
| C10—C11—C12 | 121.1 (2) | C25—C24—H23 | 120.6 |
| C10—C11—H11 | 119.5 | C24—C25—C20 | 123.31 (17) |
| C12—C11—H11 | 119.5 | C24—C25—N3 | 115.63 (15) |
| C13—C12—C11 | 122.2 (2) | C20—C25—N3 | 121.01 (16) |
| C13—C12—H12 | 118.9 | C14—N1—C7 | 107.57 (13) |
| C11—C12—H12 | 118.9 | C14—N1—S1 | 120.91 (11) |
| C12—C13—C14 | 116.9 (2) | C7—N1—S1 | 123.89 (12) |
| C12—C13—H13 | 121.5 | O6—N3—O5 | 122.39 (18) |
| C14—C13—H13 | 121.5 | O6—N3—C25 | 118.61 (16) |
| C13—C14—C9 | 121.65 (19) | O5—N3—C25 | 118.88 (16) |
| C13—C14—N1 | 130.80 (18) | O1—S1—O2 | 120.22 (10) |
| C9—C14—N1 | 107.55 (14) | O1—S1—N1 | 106.22 (8) |
| O3—C15—C16 | 122.04 (18) | O2—S1—N1 | 106.01 (9) |
| O3—C15—C8 | 119.14 (17) | O1—S1—C1 | 109.63 (10) |
| C16—C15—C8 | 118.71 (16) | O2—S1—C1 | 109.04 (10) |
| C15—C16—C17 | 114.9 (2) | N1—S1—C1 | 104.52 (8) |
| C15—C16—H16A | 108.5 | | |

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|---|---|---|---|
| C6—C1—C2—C3 | −1.9 (4) | C25—C20—C21—C22 | 0.3 (3) |
| S1—C1—C2—C3 | −178.8 (2) | C19—C20—C21—C22 | 177.18 (19) |
| C1—C2—C3—C4 | −1.3 (5) | C20—C21—C22—C23 | −1.1 (3) |
| C2—C3—C4—C5 | 3.6 (5) | C21—C22—C23—C24 | 1.4 (3) |

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|---|---|---|---|
| C3—C4—C5—C6 | −2.7 (5) | C21—C22—C23—Cl1 | −179.18 (17) |
| C2—C1—C6—C5 | 2.7 (4) | C22—C23—C24—C25 | −0.7 (3) |
| S1—C1—C6—C5 | 179.7 (2) | Cl1—C23—C24—C25 | 179.79 (14) |
| C4—C5—C6—C1 | −0.4 (5) | C23—C24—C25—C20 | −0.1 (3) |
| N1—C7—C8—C9 | −1.87 (19) | C23—C24—C25—N3 | 177.42 (17) |
| C18—C7—C8—C9 | 179.19 (17) | C21—C20—C25—C24 | 0.4 (3) |
| N1—C7—C8—C15 | 174.39 (17) | C19—C20—C25—C24 | −176.37 (17) |
| C18—C7—C8—C15 | −4.6 (3) | C21—C20—C25—N3 | −177.05 (18) |
| C7—C8—C9—C10 | 179.8 (2) | C19—C20—C25—N3 | 6.2 (3) |
| C15—C8—C9—C10 | 3.2 (3) | C13—C14—N1—C7 | 179.4 (2) |
| C7—C8—C9—C14 | 0.9 (2) | C9—C14—N1—C7 | −1.50 (18) |
| C15—C8—C9—C14 | −175.62 (16) | C13—C14—N1—S1 | 28.8 (3) |
| C14—C9—C10—C11 | −1.5 (3) | C9—C14—N1—S1 | −152.11 (13) |
| C8—C9—C10—C11 | 179.8 (2) | C8—C7—N1—C14 | 2.11 (19) |
| C9—C10—C11—C12 | 1.6 (4) | C18—C7—N1—C14 | −178.85 (15) |
| C10—C11—C12—C13 | −0.7 (4) | C8—C7—N1—S1 | 151.63 (13) |
| C11—C12—C13—C14 | −0.3 (4) | C18—C7—N1—S1 | −29.3 (2) |
| C12—C13—C14—C9 | 0.4 (3) | C24—C25—N3—O6 | −155.4 (2) |
| C12—C13—C14—N1 | 179.3 (2) | C20—C25—N3—O6 | 22.2 (3) |
| C10—C9—C14—C13 | 0.5 (3) | C24—C25—N3—O5 | 20.7 (3) |
| C8—C9—C14—C13 | 179.57 (18) | C20—C25—N3—O5 | −161.72 (19) |
| C10—C9—C14—N1 | −178.64 (17) | C14—N1—S1—O1 | −178.89 (13) |
| C8—C9—C14—N1 | 0.39 (19) | C7—N1—S1—O1 | 35.43 (16) |
| C7—C8—C15—O3 | 121.1 (3) | C14—N1—S1—O2 | −49.93 (15) |
| C9—C8—C15—O3 | −63.1 (3) | C7—N1—S1—O2 | 164.38 (14) |
| C7—C8—C15—C16 | −62.5 (3) | C14—N1—S1—C1 | 65.22 (15) |
| C9—C8—C15—C16 | 113.3 (2) | C7—N1—S1—C1 | −80.47 (15) |
| O3—C15—C16—C17 | 6.7 (4) | C6—C1—S1—O1 | −37.0 (2) |
| C8—C15—C16—C17 | −169.6 (2) | C2—C1—S1—O1 | 139.98 (19) |
| C8—C7—C18—C19 | −39.8 (3) | C6—C1—S1—O2 | −170.50 (19) |
| N1—C7—C18—C19 | 141.39 (18) | C2—C1—S1—O2 | 6.5 (2) |
| C7—C18—C19—C20 | −178.51 (16) | C6—C1—S1—N1 | 76.5 (2) |
| C18—C19—C20—C21 | 37.1 (3) | C2—C1—S1—N1 | −106.5 (2) |
| C18—C19—C20—C25 | −146.33 (19) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10···O1$^{i}$ | 0.93 | 2.60 | 3.327 (3) | 136 |
| C16—H16*B*···O5$^{ii}$ | 0.97 | 2.37 | 3.260 (3) | 152 |

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