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# Ethyl 1-benzenesulfonyl-2-[(*E*)-2-(2-methylphenyl)ethenyl]indole-3-carboxylate

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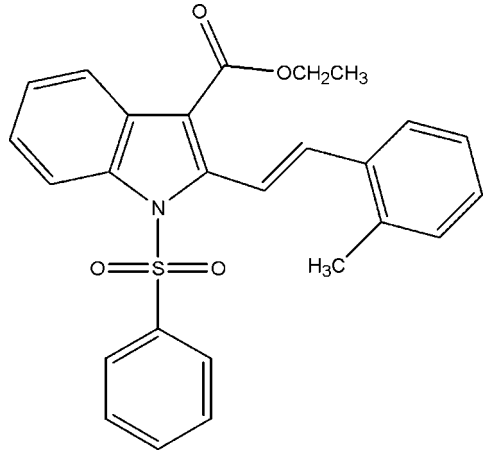
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.042; $wR$ factor = 0.117; data-to-parameter ratio = 16.7.

In the title compound, $C_{26}H_{23}NO_4S$, the phenyl, tolyl and ester groups make dihedral angles of 82.28 (5), 77.67 (6) and 8.52 (6)°, respectively, with the indole ring system. The S atom of the sulfonyl group is displaced by 0.1968 (4) Å from the indole mean plane. The molecular structure is stabilized by weak intramolecular C—H···O interactions. The crystal structure structure features short intramolecular C—H···O contacts and $\pi$–$\pi$ stacking interactions between the phenyl and tolyl groups [centroid–centroid distance = 3.9448 (11) Å].

## Related literature

For the biological activity of indole derivatives, see: Andreani *et al.* (2001); Kolocouris *et al.* (1994); Merck (1973). For the structures of closely related compounds, see: Chakkaravarthi *et al.* (2007, 2008).




## Experimental

### Crystal data

$C_{26}H_{23}NO_4S$
$M_r$ = 445.51
Monoclinic, $P2_1/n$
$a$ = 10.4248 (4) Å
$b$ = 8.3629 (3) Å
$c$ = 25.2284 (11) Å
$\beta$ = 92.902 (1)°
$V$ = 2196.63 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 295 K
0.24 × 0.20 × 0.18 mm

### Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.958, $T_{max}$ = 0.968
22952 measured reflections
4848 independent reflections
3551 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
$S$ = 1.03
4848 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···O3 | 0.93 | 2.48 | 3.000 (3) | 116 |
| C13—H13···O1 | 0.93 | 2.33 | 2.908 (3) | 120 |
| C16—H16$A$···O1$^{i}$ | 0.97 | 2.56 | 3.381 (3) | 143 |

Symmetry code: (i) $x-1, y, z$.

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*.

CR wishes to acknowledge AMET University management, India, for their kind support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2338).

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# supporting information

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## Ethyl 1-benzenesulfonyl-2-[(*E*)-2-(2-methylphenyl)ethenyl]indole-3-carboxylate

**C. Ramathilagam, V. Saravanan, A. K. Mohanakrishnan, G. Chakkaravarthi, P. R. Umarani and V. Manivannan**

### S1. Comment

Indole derivatives exhibit antihypertensive (Merck, 1973), antitumour (Andreani *et al.*, 2001) and antiviral (Kolocouris *et al.*, 1994) activities. The geometric parameters of the title molecule (Fig. 1) agree well with the reported similar structures (Chakkaravarthi *et al.* 2007, 2008).

The phenyl ring makes the dihedral angle of 82.28 (5)° with the indole ring system. The benzene ring (C20—C25) forms the dihedral angle of 77.67 (6)° with the indole ring system. The S atom of the sulfonyl group is displaced 0.1968 (4)Å from the indole mean plane. The sum of the bond angles around N1 [358.5 (1)°] indicates that N1 atom is $sp^2$ hybridized. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing exhibits weak intermolecular C—H···O (Fig.2 and Table 1) and $\pi$–$\pi$ interactions [*Cg*2···*Cg*4 (1/2 - *x*,-1/2 + *y*,1/2 - *z*) distance of 3.9448 (11) Å; *Cg*2 and *Cg*4 are the centroids of C1—C6 ring and C20—C26 ring, respectively] .

### S2. Experimental

To a suspension of hexane (5 ml) washed NaH (0.29 g, 6.10 mmol) in dry THF (10 ml) at -10° C under $N_2$ atmosphere was slowly added the solution of diethyl (3-(ethoxycarbonyl)-1-phenylsulfonyl-1*H*-indol-2-yl)methylphosphonate (0.97 g, 2.03 mmol) in dry THF (5 ml) *via* syringe and stirred for 15 min. Then a solution of 2-methylbenzaldehyde (0.28 g, 2.32 mmol) in dry THF (5 ml) was added and allowed to stir for additional 2 h. After completion of the product formation (monitored by TLC), it was then poured over crushed ice (100 g) containing conc. HCl (3 ml). The solid formed was filtered and recrystalized with MeOH to afford ethyl 2-(2-methylstyryl)-1-phenylsulfonyl -1*H*-indole-3-carboxylate as bright yellow crystals [0.70 g, 78%; melting point 371–373 K].

### S3. Refinement

H atoms were positioned geometrically and refined using riding model approximation with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic C—H and C—H = 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for methylene group and C—H = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl group.

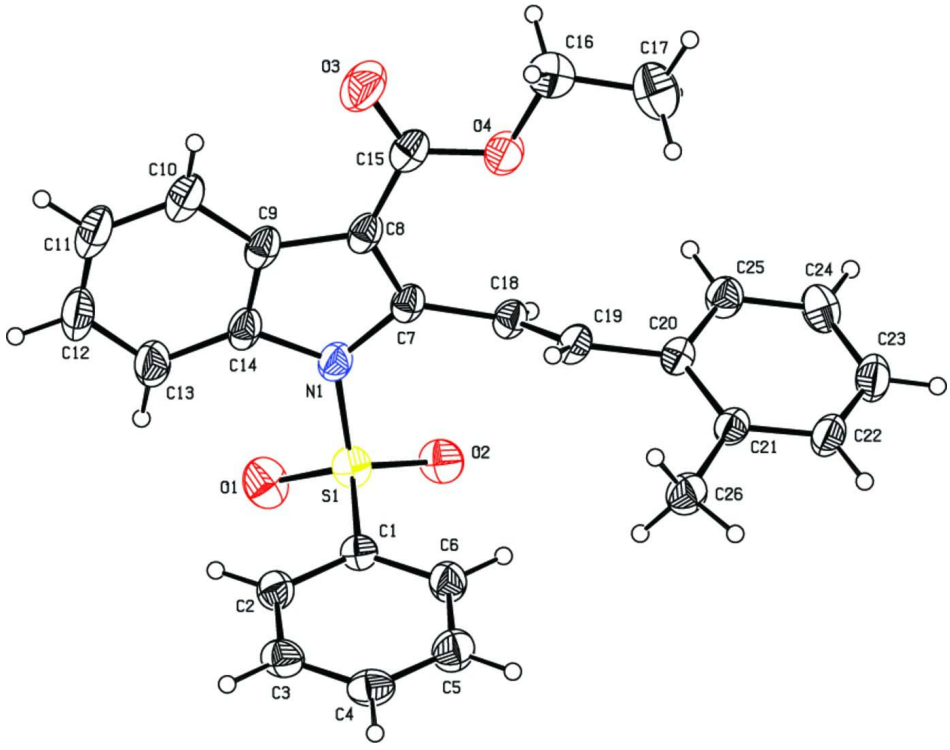


**Figure 1**

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

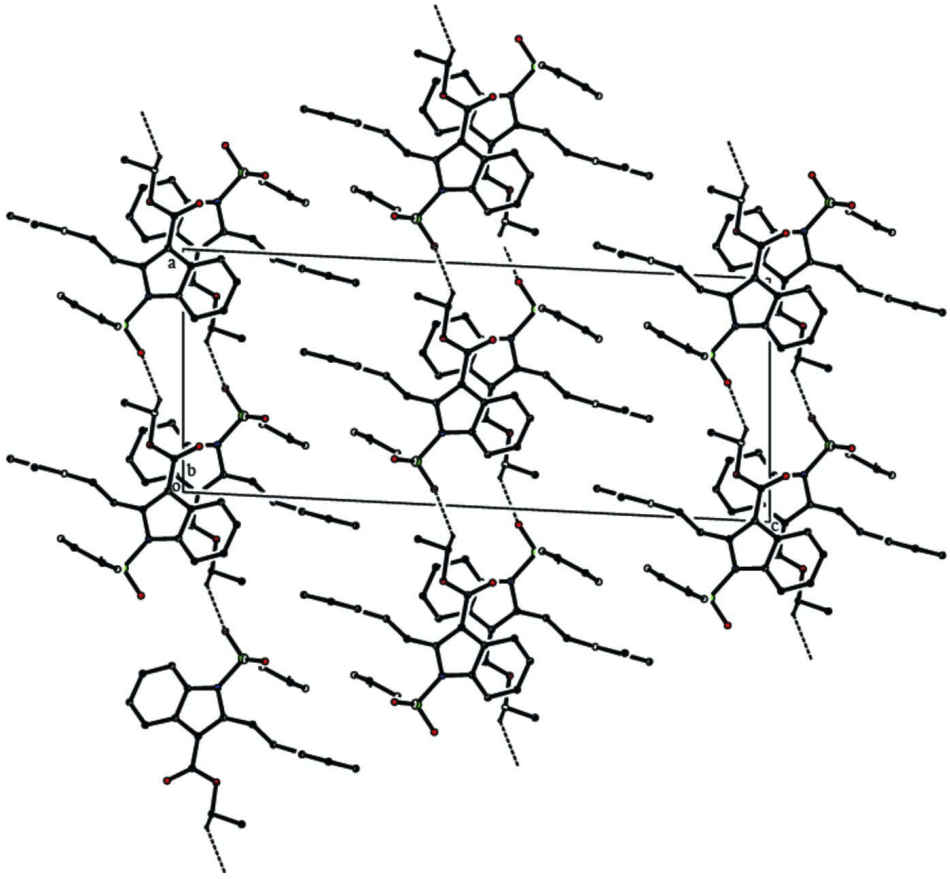


**Figure 2**

The crystal packing viewed down the *b* axis. Intermolecular C-H···O interactionshydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

### Ethyl 1-benzenesulfonyl-2-[(*E*)-2-(2-methylphenyl)ethenyl]indole-3-carboxylate

*Crystal data*

$C_{26}H_{23}NO_4S$
$M_r = 445.51$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.4248\ (4)$ Å
$b = 8.3629\ (3)$ Å
$c = 25.2284\ (11)$ Å
$\beta = 92.902\ (1)°$
$V = 2196.63\ (15)$ Å$^3$
$Z = 4$
$F(000) = 936$
$D_x = 1.347$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 31039 reflections
$\theta = 2.1–31.4°$
$\mu = 0.18$ mm$^{-1}$
$T = 295$ K
Block, yellow
0.24 × 0.20 × 0.18 mm

*Data collection*

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.958$, $T_{max} = 0.968$
22952 measured reflections
4848 independent reflections
3551 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.029
$\theta_{max}$ = 27.1°, $\theta_{min}$ = 2.1°
$h$ = −12→13
$k$ = −10→10
$l$ = −32→32

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
$S$ = 1.03
4848 reflections
291 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
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.6907P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.29596 (16) | 0.5477 (2) | 0.13482 (7) | 0.0434 (4) |
| C2 | 0.33149 (19) | 0.4055 (2) | 0.11194 (7) | 0.0516 (4) |
| H2 | 0.3705 | 0.4051 | 0.0796 | 0.062* |
| C3 | 0.3082 (2) | 0.2640 (2) | 0.13788 (8) | 0.0563 (5) |
| H3 | 0.3314 | 0.1672 | 0.1229 | 0.068* |
| C4 | 0.2511 (2) | 0.2656 (2) | 0.18551 (8) | 0.0582 (5) |
| H4 | 0.2353 | 0.1697 | 0.2027 | 0.070* |
| C5 | 0.2170 (2) | 0.4074 (3) | 0.20820 (8) | 0.0641 (6) |
| H5 | 0.1793 | 0.4073 | 0.2408 | 0.077* |
| C6 | 0.23856 (19) | 0.5502 (2) | 0.18277 (8) | 0.0549 (5) |
| H6 | 0.2147 | 0.6466 | 0.1978 | 0.066* |
| C7 | 0.07971 (18) | 0.81521 (19) | 0.06872 (6) | 0.0439 (4) |
| C8 | −0.00146 (19) | 0.7883 (2) | 0.02544 (6) | 0.0466 (4) |
| C9 | 0.0676 (2) | 0.7013 (2) | −0.01332 (7) | 0.0505 (5) |
| C10 | 0.0332 (2) | 0.6438 (2) | −0.06437 (7) | 0.0644 (6) |
| H10 | −0.0487 | 0.6611 | −0.0796 | 0.077* |
| C11 | 0.1231 (3) | 0.5617 (3) | −0.09121 (9) | 0.0782 (8) |
| H11 | 0.1019 | 0.5246 | −0.1253 | 0.094* |
| C12 | 0.2444 (3) | 0.5327 (3) | −0.06897 (9) | 0.0803 (8) |
| H12 | 0.3020 | 0.4733 | −0.0879 | 0.096* |
| C13 | 0.2824 (3) | 0.5898 (3) | −0.01920 (8) | 0.0698 (6) |
| H13 | 0.3647 | 0.5719 | −0.0045 | 0.084* |
| C14 | 0.1920 (2) | 0.6752 (2) | 0.00782 (7) | 0.0530 (5) |
| C15 | −0.1351 (2) | 0.8425 (2) | 0.01525 (7) | 0.0520 (5) |
| C16 | −0.3192 (2) | 0.9600 (3) | 0.04901 (9) | 0.0683 (6) |
| H16A | −0.3749 | 0.8700 | 0.0401 | 0.082* |
| H16B | −0.3273 | 1.0375 | 0.0204 | 0.082* |
| C17 | −0.3556 (3) | 1.0338 (3) | 0.09964 (11) | 0.0900 (8) |
| H17A | −0.2996 | 1.1223 | 0.1081 | 0.135* |
| H17B | −0.3479 | 0.9558 | 0.1275 | 0.135* |
| H17C | −0.4427 | 1.0710 | 0.0960 | 0.135* |

| | | | | |
|---|---|---|---|---|
| C18 | 0.05757 (17) | 0.9015 (2) | 0.11824 (6) | 0.0458 (4) |
| H18 | 0.1021 | 0.9965 | 0.1247 | 0.055* |
| C19 | −0.02112 (18) | 0.8527 (2) | 0.15390 (6) | 0.0479 (4) |
| H19 | −0.0617 | 0.7549 | 0.1479 | 0.057* |
| C20 | −0.05081 (16) | 0.9393 (2) | 0.20259 (7) | 0.0445 (4) |
| C21 | −0.07577 (16) | 0.8570 (2) | 0.24966 (6) | 0.0460 (4) |
| C22 | −0.10097 (19) | 0.9451 (3) | 0.29430 (7) | 0.0570 (5) |
| H22 | −0.1176 | 0.8917 | 0.3255 | 0.068* |
| C23 | −0.1022 (2) | 1.1089 (3) | 0.29386 (8) | 0.0644 (6) |
| H23 | −0.1181 | 1.1652 | 0.3246 | 0.077* |
| C24 | −0.0800 (2) | 1.1895 (3) | 0.24804 (9) | 0.0644 (6) |
| H24 | −0.0816 | 1.3007 | 0.2475 | 0.077* |
| C25 | −0.05529 (19) | 1.1053 (2) | 0.20262 (8) | 0.0543 (5) |
| H25 | −0.0414 | 1.1607 | 0.1715 | 0.065* |
| C26 | −0.0706 (2) | 0.6777 (2) | 0.25305 (8) | 0.0594 (5) |
| H26A | −0.0929 | 0.6442 | 0.2878 | 0.089* |
| H26B | 0.0146 | 0.6417 | 0.2465 | 0.089* |
| H26C | −0.1304 | 0.6326 | 0.2270 | 0.089* |
| N1 | 0.20131 (15) | 0.75147 (17) | 0.05839 (6) | 0.0494 (4) |
| O1 | 0.43527 (14) | 0.70935 (19) | 0.07195 (6) | 0.0717 (4) |
| O2 | 0.31983 (13) | 0.85612 (15) | 0.13962 (5) | 0.0603 (4) |
| O3 | −0.19140 (16) | 0.8300 (2) | −0.02733 (6) | 0.0866 (5) |
| O4 | −0.18768 (13) | 0.90745 (18) | 0.05650 (5) | 0.0618 (4) |
| S1 | 0.32570 (5) | 0.72867 (5) | 0.10266 (2) | 0.05081 (15) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0433 (9) | 0.0401 (8) | 0.0464 (9) | −0.0039 (7) | −0.0009 (7) | 0.0010 (7) |
| C2 | 0.0587 (12) | 0.0467 (10) | 0.0492 (10) | 0.0004 (8) | 0.0014 (9) | −0.0044 (8) |
| C3 | 0.0654 (13) | 0.0397 (9) | 0.0624 (12) | 0.0005 (9) | −0.0099 (10) | −0.0035 (8) |
| C4 | 0.0644 (13) | 0.0464 (10) | 0.0625 (12) | −0.0059 (9) | −0.0087 (10) | 0.0116 (9) |
| C5 | 0.0771 (15) | 0.0591 (12) | 0.0571 (12) | −0.0003 (11) | 0.0132 (10) | 0.0104 (10) |
| C6 | 0.0661 (12) | 0.0454 (10) | 0.0538 (11) | 0.0034 (9) | 0.0104 (9) | 0.0007 (8) |
| C7 | 0.0591 (11) | 0.0362 (8) | 0.0371 (8) | −0.0067 (8) | 0.0108 (8) | 0.0032 (7) |
| C8 | 0.0653 (12) | 0.0390 (9) | 0.0363 (9) | −0.0110 (8) | 0.0094 (8) | 0.0019 (7) |
| C9 | 0.0780 (14) | 0.0366 (9) | 0.0380 (9) | −0.0125 (9) | 0.0134 (9) | 0.0027 (7) |
| C10 | 0.1043 (17) | 0.0483 (11) | 0.0412 (10) | −0.0157 (11) | 0.0112 (10) | −0.0031 (9) |
| C11 | 0.146 (3) | 0.0495 (12) | 0.0414 (11) | −0.0110 (14) | 0.0231 (14) | −0.0058 (9) |
| C12 | 0.139 (2) | 0.0523 (12) | 0.0534 (13) | 0.0117 (14) | 0.0431 (15) | 0.0011 (10) |
| C13 | 0.0991 (17) | 0.0592 (12) | 0.0537 (12) | 0.0121 (12) | 0.0293 (12) | 0.0066 (10) |
| C14 | 0.0827 (14) | 0.0383 (9) | 0.0396 (9) | −0.0030 (9) | 0.0199 (9) | 0.0045 (7) |
| C15 | 0.0654 (12) | 0.0482 (10) | 0.0426 (10) | −0.0170 (9) | 0.0037 (9) | 0.0007 (8) |
| C16 | 0.0565 (13) | 0.0702 (14) | 0.0784 (15) | −0.0075 (11) | 0.0065 (11) | 0.0081 (12) |
| C17 | 0.0768 (17) | 0.0912 (18) | 0.104 (2) | 0.0034 (14) | 0.0249 (15) | −0.0120 (16) |
| C18 | 0.0572 (11) | 0.0414 (9) | 0.0389 (9) | −0.0050 (8) | 0.0039 (8) | −0.0034 (7) |
| C19 | 0.0635 (12) | 0.0429 (9) | 0.0376 (9) | −0.0074 (8) | 0.0051 (8) | −0.0013 (7) |
| C20 | 0.0440 (10) | 0.0504 (10) | 0.0390 (9) | −0.0034 (8) | 0.0024 (7) | −0.0036 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 0.0398 (9) | 0.0587 (11) | 0.0394 (9) | −0.0019 (8) | 0.0019 (7) | −0.0001 (8) |
| C22 | 0.0562 (12) | 0.0771 (14) | 0.0380 (9) | 0.0023 (10) | 0.0074 (8) | −0.0026 (9) |
| C23 | 0.0654 (13) | 0.0780 (15) | 0.0504 (11) | 0.0045 (11) | 0.0079 (10) | −0.0189 (11) |
| C24 | 0.0672 (14) | 0.0521 (11) | 0.0745 (14) | 0.0019 (10) | 0.0106 (11) | −0.0151 (10) |
| C25 | 0.0615 (12) | 0.0514 (10) | 0.0507 (10) | −0.0026 (9) | 0.0085 (9) | 0.0002 (9) |
| C26 | 0.0654 (13) | 0.0607 (12) | 0.0528 (11) | −0.0022 (10) | 0.0115 (10) | 0.0078 (9) |
| N1 | 0.0647 (10) | 0.0456 (8) | 0.0386 (8) | 0.0016 (7) | 0.0102 (7) | 0.0027 (6) |
| O1 | 0.0589 (9) | 0.0704 (10) | 0.0881 (11) | −0.0103 (7) | 0.0267 (8) | 0.0072 (8) |
| O2 | 0.0694 (9) | 0.0408 (7) | 0.0699 (9) | −0.0097 (6) | −0.0036 (7) | −0.0054 (6) |
| O3 | 0.0824 (11) | 0.1226 (15) | 0.0535 (9) | −0.0018 (10) | −0.0107 (8) | −0.0151 (9) |
| O4 | 0.0587 (9) | 0.0764 (9) | 0.0504 (8) | 0.0003 (7) | 0.0037 (6) | −0.0047 (7) |
| S1 | 0.0530 (3) | 0.0423 (2) | 0.0579 (3) | −0.0081 (2) | 0.0101 (2) | 0.0021 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.377 (3) | C15—O4 | 1.318 (2) |
| C1—C2 | 1.381 (2) | C16—O4 | 1.444 (2) |
| C1—S1 | 1.7523 (17) | C16—C17 | 1.485 (3) |
| C2—C3 | 1.379 (3) | C16—H16A | 0.9700 |
| C2—H2 | 0.9300 | C16—H16B | 0.9700 |
| C3—C4 | 1.368 (3) | C17—H17A | 0.9600 |
| C3—H3 | 0.9300 | C17—H17B | 0.9600 |
| C4—C5 | 1.371 (3) | C17—H17C | 0.9600 |
| C4—H4 | 0.9300 | C18—C19 | 1.313 (2) |
| C5—C6 | 1.379 (3) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—C20 | 1.472 (2) |
| C6—H6 | 0.9300 | C19—H19 | 0.9300 |
| C7—C8 | 1.366 (2) | C20—C25 | 1.389 (3) |
| C7—N1 | 1.412 (2) | C20—C21 | 1.408 (2) |
| C7—C18 | 1.471 (2) | C21—C22 | 1.382 (3) |
| C8—C9 | 1.440 (2) | C21—C26 | 1.503 (3) |
| C8—C15 | 1.475 (3) | C22—C23 | 1.370 (3) |
| C9—C14 | 1.394 (3) | C22—H22 | 0.9300 |
| C9—C10 | 1.404 (3) | C23—C24 | 1.368 (3) |
| C10—C11 | 1.368 (3) | C23—H23 | 0.9300 |
| C10—H10 | 0.9300 | C24—C25 | 1.380 (3) |
| C11—C12 | 1.379 (4) | C24—H24 | 0.9300 |
| C11—H11 | 0.9300 | C25—H25 | 0.9300 |
| C12—C13 | 1.383 (3) | C26—H26A | 0.9600 |
| C12—H12 | 0.9300 | C26—H26B | 0.9600 |
| C13—C14 | 1.388 (3) | C26—H26C | 0.9600 |
| C13—H13 | 0.9300 | N1—S1 | 1.6789 (17) |
| C14—N1 | 1.425 (2) | O1—S1 | 1.4217 (14) |
| C15—O3 | 1.202 (2) | O2—S1 | 1.4194 (14) |
| | | | |
| C6—C1—C2 | 121.21 (17) | C17—C16—H16B | 110.3 |
| C6—C1—S1 | 119.25 (13) | H16A—C16—H16B | 108.5 |
| C2—C1—S1 | 119.54 (14) | C16—C17—H17A | 109.5 |

| | | | |
|---|---|---|---|
| C3—C2—C1 | 118.89 (18) | C16—C17—H17B | 109.5 |
| C3—C2—H2 | 120.6 | H17A—C17—H17B | 109.5 |
| C1—C2—H2 | 120.6 | C16—C17—H17C | 109.5 |
| C4—C3—C2 | 120.21 (18) | H17A—C17—H17C | 109.5 |
| C4—C3—H3 | 119.9 | H17B—C17—H17C | 109.5 |
| C2—C3—H3 | 119.9 | C19—C18—C7 | 124.04 (16) |
| C3—C4—C5 | 120.57 (18) | C19—C18—H18 | 118.0 |
| C3—C4—H4 | 119.7 | C7—C18—H18 | 118.0 |
| C5—C4—H4 | 119.7 | C18—C19—C20 | 125.73 (17) |
| C4—C5—C6 | 120.19 (19) | C18—C19—H19 | 117.1 |
| C4—C5—H5 | 119.9 | C20—C19—H19 | 117.1 |
| C6—C5—H5 | 119.9 | C25—C20—C21 | 118.73 (16) |
| C1—C6—C5 | 118.93 (18) | C25—C20—C19 | 120.03 (16) |
| C1—C6—H6 | 120.5 | C21—C20—C19 | 121.24 (16) |
| C5—C6—H6 | 120.5 | C22—C21—C20 | 118.50 (18) |
| C8—C7—N1 | 108.42 (15) | C22—C21—C26 | 119.57 (17) |
| C8—C7—C18 | 129.95 (17) | C20—C21—C26 | 121.89 (16) |
| N1—C7—C18 | 121.54 (16) | C23—C22—C21 | 121.92 (19) |
| C7—C8—C9 | 108.39 (18) | C23—C22—H22 | 119.0 |
| C7—C8—C15 | 129.07 (16) | C21—C22—H22 | 119.0 |
| C9—C8—C15 | 122.45 (17) | C24—C23—C22 | 119.83 (19) |
| C14—C9—C10 | 119.08 (19) | C24—C23—H23 | 120.1 |
| C14—C9—C8 | 107.85 (16) | C22—C23—H23 | 120.1 |
| C10—C9—C8 | 133.1 (2) | C23—C24—C25 | 119.8 (2) |
| C11—C10—C9 | 118.5 (2) | C23—C24—H24 | 120.1 |
| C11—C10—H10 | 120.8 | C25—C24—H24 | 120.1 |
| C9—C10—H10 | 120.8 | C24—C25—C20 | 121.19 (19) |
| C10—C11—C12 | 121.6 (2) | C24—C25—H25 | 119.4 |
| C10—C11—H11 | 119.2 | C20—C25—H25 | 119.4 |
| C12—C11—H11 | 119.2 | C21—C26—H26A | 109.5 |
| C11—C12—C13 | 121.6 (2) | C21—C26—H26B | 109.5 |
| C11—C12—H12 | 119.2 | H26A—C26—H26B | 109.5 |
| C13—C12—H12 | 119.2 | C21—C26—H26C | 109.5 |
| C12—C13—C14 | 116.9 (2) | H26A—C26—H26C | 109.5 |
| C12—C13—H13 | 121.5 | H26B—C26—H26C | 109.5 |
| C14—C13—H13 | 121.5 | C7—N1—C14 | 108.25 (16) |
| C13—C14—C9 | 122.30 (19) | C7—N1—S1 | 126.20 (12) |
| C13—C14—N1 | 130.7 (2) | C14—N1—S1 | 124.06 (14) |
| C9—C14—N1 | 106.99 (16) | C15—O4—C16 | 116.92 (16) |
| O3—C15—O4 | 122.5 (2) | O2—S1—O1 | 120.39 (9) |
| O3—C15—C8 | 122.88 (19) | O2—S1—N1 | 107.11 (8) |
| O4—C15—C8 | 114.58 (16) | O1—S1—N1 | 105.37 (9) |
| O4—C16—C17 | 107.22 (19) | O2—S1—C1 | 109.27 (8) |
| O4—C16—H16A | 110.3 | O1—S1—C1 | 108.67 (9) |
| C17—C16—H16A | 110.3 | N1—S1—C1 | 104.91 (8) |
| O4—C16—H16B | 110.3 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.2 (3) | C18—C19—C20—C21 | −146.01 (19) |

| | | | |
|---|---|---|---|
| S1—C1—C2—C3 | 179.60 (15) | C25—C20—C21—C22 | −1.4 (3) |
| C1—C2—C3—C4 | −0.2 (3) | C19—C20—C21—C22 | 178.96 (17) |
| C2—C3—C4—C5 | −0.4 (3) | C25—C20—C21—C26 | −178.99 (18) |
| C3—C4—C5—C6 | 0.8 (3) | C19—C20—C21—C26 | 1.4 (3) |
| C2—C1—C6—C5 | 0.3 (3) | C20—C21—C22—C23 | 0.0 (3) |
| S1—C1—C6—C5 | −179.13 (16) | C26—C21—C22—C23 | 177.64 (19) |
| C4—C5—C6—C1 | −0.8 (3) | C21—C22—C23—C24 | 1.0 (3) |
| N1—C7—C8—C9 | 1.62 (18) | C22—C23—C24—C25 | −0.6 (3) |
| C18—C7—C8—C9 | 178.34 (16) | C23—C24—C25—C20 | −0.8 (3) |
| N1—C7—C8—C15 | −174.87 (16) | C21—C20—C25—C24 | 1.8 (3) |
| C18—C7—C8—C15 | 1.8 (3) | C19—C20—C25—C24 | −178.52 (18) |
| C7—C8—C9—C14 | 0.51 (19) | C8—C7—N1—C14 | −3.13 (18) |
| C15—C8—C9—C14 | 177.28 (15) | C18—C7—N1—C14 | 179.82 (14) |
| C7—C8—C9—C10 | −179.41 (18) | C8—C7—N1—S1 | −169.56 (12) |
| C15—C8—C9—C10 | −2.6 (3) | C18—C7—N1—S1 | 13.4 (2) |
| C14—C9—C10—C11 | 1.0 (3) | C13—C14—N1—C7 | −177.09 (18) |
| C8—C9—C10—C11 | −179.08 (19) | C9—C14—N1—C7 | 3.40 (18) |
| C9—C10—C11—C12 | 1.0 (3) | C13—C14—N1—S1 | −10.3 (3) |
| C10—C11—C12—C13 | −2.2 (4) | C9—C14—N1—S1 | 170.19 (12) |
| C11—C12—C13—C14 | 1.2 (3) | O3—C15—O4—C16 | 1.7 (3) |
| C12—C13—C14—C9 | 0.9 (3) | C8—C15—O4—C16 | −178.92 (16) |
| C12—C13—C14—N1 | −178.54 (18) | C17—C16—O4—C15 | −177.89 (18) |
| C10—C9—C14—C13 | −2.0 (3) | C7—N1—S1—O2 | −32.90 (16) |
| C8—C9—C14—C13 | 178.05 (17) | C14—N1—S1—O2 | 162.70 (14) |
| C10—C9—C14—N1 | 177.54 (15) | C7—N1—S1—O1 | −162.21 (14) |
| C8—C9—C14—N1 | −2.39 (18) | C14—N1—S1—O1 | 33.38 (16) |
| C7—C8—C15—O3 | 169.53 (19) | C7—N1—S1—C1 | 83.16 (15) |
| C9—C8—C15—O3 | −6.5 (3) | C14—N1—S1—C1 | −81.24 (15) |
| C7—C8—C15—O4 | −9.8 (3) | C6—C1—S1—O2 | 17.63 (18) |
| C9—C8—C15—O4 | 174.12 (15) | C2—C1—S1—O2 | −161.76 (15) |
| C8—C7—C18—C19 | 67.2 (3) | C6—C1—S1—O1 | 150.76 (16) |
| N1—C7—C18—C19 | −116.4 (2) | C2—C1—S1—O1 | −28.63 (18) |
| C7—C18—C19—C20 | −176.79 (17) | C6—C1—S1—N1 | −96.93 (16) |
| C18—C19—C20—C25 | 34.3 (3) | C2—C1—S1—N1 | 83.68 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10···O3 | 0.93 | 2.48 | 3.000 (3) | 116 |
| C13—H13···O1 | 0.93 | 2.33 | 2.908 (3) | 120 |
| C16—H16*A*···O1$^{i}$ | 0.97 | 2.56 | 3.381 (3) | 143 |

Symmetry code: (i) *x*−1, *y*, *z*.