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# Crystal structure of (*E*)-diethyl 2-[(1-phenylsulfonyl-1*H*-indol-3-yl)methylidene]succinate

**M. Umadevi,[a,b] Potharaju Raju,[c] R. Yamuna,[d]* Arasambattu K. Mohanakrishnan[c] and G. Chakkaravarthi[e]***

[a]Research and Development Centre, Bharathiar University, Coimbatore 641 046, India, [b]Department of Chemistry, Pallavan College of Engineering, Kanchipuram 631 502, India, [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, [d]Department of Sciences, Chemistry and Materials Research Lab, Amrita Vishwa Vidyapeetham University, Ettimadai, Coimbatore 641 112, India, and [e]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India. *Correspondence e-mail: ryamuna1@gmail.com, chakkaravarthi_2005@yahoo.com

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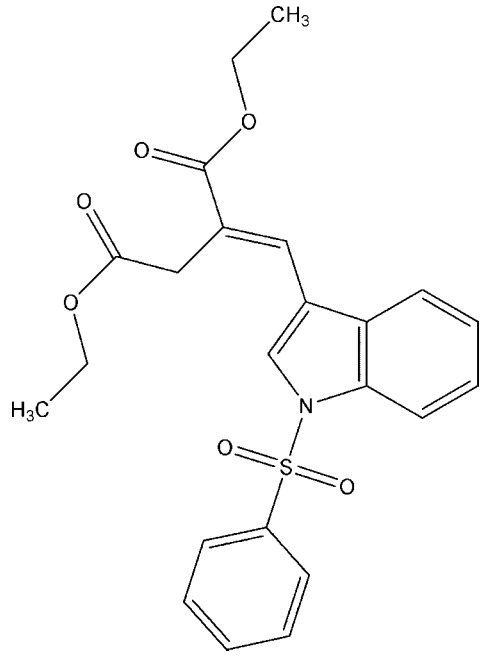
In the title compound, $C_{23}H_{23}NO_6S$, the phenyl ring is perpendicular [dihedral angle = 89.34 (9)°] to the indole ring system. In the molecule, the ethoxy groups are each disordered over two sets of sites with occupancy ratios of 0.671 (6):0.329 (6) and 0.75 (3):0.25 (3). The molecular conformation is consolidated by a weak C—H···O interaction, which generates an $S(6)$ graph–set motif. The packing of the molecules in the crystal structure features weak C—H···$\pi$ interactions.

**Keywords:** crystal structure; indole derivative; hydrogen bonding.

**CCDC reference**: 1439879

## 1. Related literature

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



## 2. Experimental

### 2.1. Crystal data

$C_{23}H_{23}NO_6S$
$M_r$ = 441.48
Monoclinic, $P2_1/n$
$a$ = 8.3458 (8) Å
$b$ = 24.657 (2) Å
$c$ = 10.9448 (9) Å
$\beta$ = 91.121 (3)°
$V$ = 2251.8 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 295 K
0.30 × 0.24 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.947, $T_{max}$ = 0.965
31225 measured reflections
4631 independent reflections
2889 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.139
$S$ = 1.03
4631 reflections
322 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

*Cg*2 is the centroid of C1–C6 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13···O1 | 0.93 | 2.44 | 3.012 (4) | 120 |
| C12—H12···*Cg*2$^{i}$ | 0.93 | 2.80 | 3.561 (4) | 140 |

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

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*.

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RK2433).

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# supporting information

*Acta Cryst.* (2015). E**71**, o1029–o1030 [https://doi.org/10.1107/S2056989015023075]

## Crystal structure of (*E*)-diethyl 2-[(1-phenylsulfonyl-1*H*-indol-3-yl)methylidene]succinate

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

### S1. Structural commentary

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

The phenyl ring (C1–C6) is perpendicular [dihedral angle of 89.34 (9)°] to indole ring (N1/C7–C14) system in the molecule. In the terminal site, the ethoxy group is disordered over two positions with site occupancies of 0.671 (6) for major component (O4/C19/C20) and 0.329 (6) for minor component (O4A/C19A/C20A). The other ethoxy group is also disordered over two positions with site occupancies of 0.75 (3) for major component (O6/C23/C24) and 0.25 (3) for minor component (O6A/C23A/C24A). The torsion angles O1—S1—N1—C14 and O2—S1—N1—C7 [39.9 (2)° and -32.8 (2)°, respectively] indicate the syn–conformation of the sulfonyl moiety. The molecular structure is stabilized by weak non–classical C—H···O hydrogen bond which generates S(6) graph–set (Table 1 & Fig. 1) motif. The crystal structure is influenced by weak C—H···$\pi$ (Table 1) interactions in a three–dimensional network.

### S2. Synthesis and crystallization

To a solution of 1–(phenylsulfonyl)–1*H*–indole–3–carboxaldehyde (0.5 g, 1.84 mmol) and phosphorous ylide ($C_{26}H_{27}O_4P$) (0.96 g, 2.21 mmol) [prepared from (carbethoxymethylene)triphenylphosphorane and ethyl bromoacetate] in dry toluene (10 ml) was refluxed for 24 h. Then the solvent was removed under reduced pressure. The solid obtained was recrystallized from methanol (3 ml) to afford the title compound as a colourless crystal suitable for X–Ray diffraction analysis.

### S3. Refinement

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

The reflections [1 2 2], [0 2 0] and [0 1 1] were omitted during refinement which were owing poor agreement. The bond distances (C19—C20), (C19A—C20A), (C22—C23) and (C22A—C23A) were restraint to 1.54 (1)Å. The anisotropic displacement parameters of terminal site disordered atoms were equalized for the major and minor components with *EADP* instruction for C20 & C20A and C19 & C19A. The anisotropic displacement parameters in the direction of S1 and O2 were restraint within 0.001 using *DELU* instruction in *SHELXL* refinement.

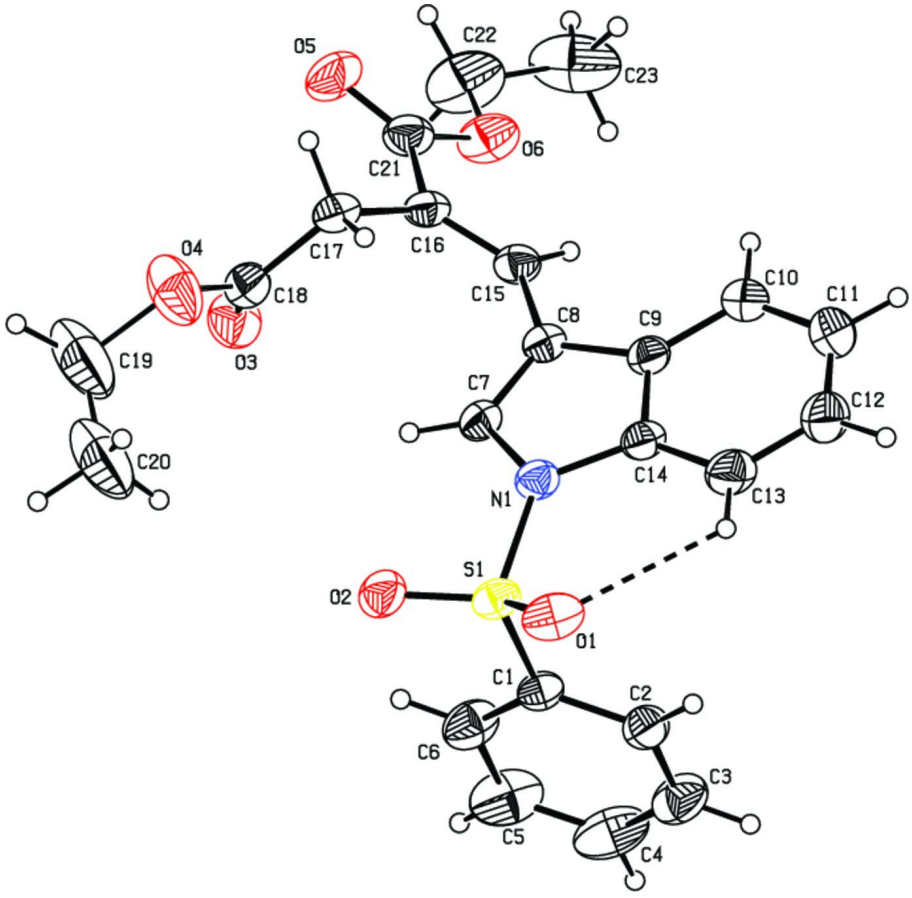


**Figure 1**

The molecular structure of title compound, with atom labels. Displacement ellipsoids are drawn at 30% probability level. The H atoms are presented as a small spheres of arbitrary radius. The minor components of the disordered ethyl groups are omitted for clarity.

**(*E*)-Diethyl 2-[(1-phenylsulfonyl-1*H*-indol-3-yl)methylidene]succinate**

*Crystal data*

$C_{23}H_{23}NO_6S$
$M_r = 441.48$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.3458\ (8)$ Å
$b = 24.657\ (2)$ Å
$c = 10.9448\ (9)$ Å
$\beta = 91.121\ (3)°$
$V = 2251.8\ (3)$ Å$^3$
$Z = 4$
$F(000) = 928$
$D_x = 1.302$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6504 reflections
$\theta = 2.5–23.4°$
$\mu = 0.18$ mm$^{-1}$
$T = 295$ K
Block, colourless
0.30 × 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)
$T_{min} = 0.947$, $T_{max} = 0.965$

31225 measured reflections
4631 independent reflections
2889 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.5°$
$h = -10 \rightarrow 10$
$k = -30 \rightarrow 30$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.139$
$S = 1.03$
4631 reflections
322 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.8923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*–factor w*R* 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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.6466 (3) | 0.30006 (9) | 0.3924 (2) | 0.0459 (6) | |
| C2 | 0.6500 (3) | 0.26226 (10) | 0.2988 (2) | 0.0567 (7) | |
| H2 | 0.7465 | 0.2522 | 0.2641 | 0.068* | |
| C3 | 0.5073 (4) | 0.23988 (12) | 0.2582 (3) | 0.0763 (9) | |
| H3 | 0.5069 | 0.2145 | 0.1953 | 0.092* | |
| C4 | 0.3674 (5) | 0.25465 (15) | 0.3095 (4) | 0.0955 (12) | |
| H4 | 0.2717 | 0.2396 | 0.2808 | 0.115* | |
| C5 | 0.3651 (4) | 0.29161 (15) | 0.4035 (4) | 0.0997 (13) | |
| H5 | 0.2686 | 0.3007 | 0.4393 | 0.120* | |
| C6 | 0.5061 (4) | 0.31516 (11) | 0.4447 (3) | 0.0715 (8) | |
| H6 | 0.5056 | 0.3408 | 0.5069 | 0.086* | |
| C7 | 0.7896 (3) | 0.43043 (9) | 0.3542 (2) | 0.0478 (6) | |
| H7 | 0.7400 | 0.4439 | 0.4232 | 0.057* | |
| C8 | 0.8039 (3) | 0.45752 (9) | 0.2475 (2) | 0.0454 (6) | |
| C9 | 0.8822 (3) | 0.42149 (9) | 0.1642 (2) | 0.0485 (6) | |
| C10 | 0.9268 (4) | 0.42694 (12) | 0.0431 (3) | 0.0663 (8) | |
| H10 | 0.9071 | 0.4590 | 0.0006 | 0.080* | |
| C11 | 1.0001 (4) | 0.38407 (14) | −0.0123 (3) | 0.0844 (10) | |
| H11 | 1.0287 | 0.3869 | −0.0937 | 0.101* | |
| C12 | 1.0325 (4) | 0.33661 (13) | 0.0507 (3) | 0.0806 (10) | |
| H12 | 1.0828 | 0.3082 | 0.0107 | 0.097* | |

| | | | | | |
|---|---|---|---|---|---|
| C13 | 0.9924 (3) | 0.33027 (11) | 0.1709 (3) | 0.0662 (8) | |
| H13 | 1.0155 | 0.2985 | 0.2134 | 0.079* | |
| C14 | 0.9159 (3) | 0.37344 (9) | 0.2258 (2) | 0.0485 (6) | |
| C15 | 0.7460 (3) | 0.51183 (9) | 0.2172 (2) | 0.0505 (6) | |
| H15 | 0.7002 | 0.5161 | 0.1396 | 0.061* | |
| C16 | 0.7508 (3) | 0.55562 (9) | 0.2867 (2) | 0.0477 (6) | |
| C17 | 0.8300 (3) | 0.55776 (10) | 0.4103 (2) | 0.0528 (7) | |
| H17A | 0.9083 | 0.5288 | 0.4167 | 0.063* | |
| H17B | 0.8869 | 0.5919 | 0.4188 | 0.063* | |
| C18 | 0.7145 (4) | 0.55251 (11) | 0.5119 (3) | 0.0588 (7) | |
| O4 | 0.7948 (8) | 0.5510 (3) | 0.6172 (6) | 0.104 (2) | 0.671 (6) |
| C19 | 0.6975 (11) | 0.5455 (4) | 0.7255 (6) | 0.152 (3) | 0.671 (6) |
| H19A | 0.5860 | 0.5536 | 0.7065 | 0.182* | 0.671 (6) |
| H19B | 0.7350 | 0.5698 | 0.7897 | 0.182* | 0.671 (6) |
| C20 | 0.7170 (10) | 0.4872 (4) | 0.7640 (6) | 0.152 (3) | 0.671 (6) |
| H20A | 0.6600 | 0.4642 | 0.7073 | 0.228* | 0.671 (6) |
| H20B | 0.6750 | 0.4824 | 0.8443 | 0.228* | 0.671 (6) |
| H20C | 0.8287 | 0.4778 | 0.7649 | 0.228* | 0.671 (6) |
| O4A | 0.7807 (15) | 0.5214 (4) | 0.6047 (10) | 0.066 (2) | 0.329 (6) |
| C19A | 0.677 (3) | 0.5038 (8) | 0.7017 (13) | 0.152 (3) | 0.329 (6) |
| H19C | 0.7058 | 0.4669 | 0.7233 | 0.182* | 0.329 (6) |
| H19D | 0.5678 | 0.5030 | 0.6694 | 0.182* | 0.329 (6) |
| C20A | 0.678 (2) | 0.5367 (8) | 0.8154 (11) | 0.152 (3) | 0.329 (6) |
| H20D | 0.7847 | 0.5369 | 0.8506 | 0.228* | 0.329 (6) |
| H20E | 0.6055 | 0.5212 | 0.8725 | 0.228* | 0.329 (6) |
| H20F | 0.6463 | 0.5731 | 0.7965 | 0.228* | 0.329 (6) |
| C21 | 0.6780 (4) | 0.60772 (11) | 0.2456 (3) | 0.0597 (7) | |
| O6 | 0.605 (2) | 0.6030 (5) | 0.1389 (16) | 0.076 (3) | 0.75 (3) |
| C22 | 0.501 (2) | 0.6514 (6) | 0.1022 (11) | 0.111 (4) | 0.75 (3) |
| H22A | 0.3980 | 0.6502 | 0.1414 | 0.133* | 0.75 (3) |
| H22B | 0.5540 | 0.6854 | 0.1226 | 0.133* | 0.75 (3) |
| C23 | 0.4834 (17) | 0.6446 (6) | −0.0316 (10) | 0.129 (5) | 0.75 (3) |
| H23A | 0.5874 | 0.6412 | −0.0668 | 0.193* | 0.75 (3) |
| H23B | 0.4293 | 0.6755 | −0.0659 | 0.193* | 0.75 (3) |
| H23C | 0.4220 | 0.6125 | −0.0490 | 0.193* | 0.75 (3) |
| O6A | 0.569 (7) | 0.6022 (18) | 0.153 (5) | 0.096 (12) | 0.25 (3) |
| C22A | 0.567 (3) | 0.6554 (16) | 0.084 (4) | 0.077 (7) | 0.25 (3) |
| H22C | 0.6598 | 0.6596 | 0.0334 | 0.093* | 0.25 (3) |
| H22D | 0.5576 | 0.6863 | 0.1384 | 0.093* | 0.25 (3) |
| C23A | 0.415 (4) | 0.6461 (18) | 0.009 (5) | 0.138 (15) | 0.25 (3) |
| H23D | 0.4365 | 0.6217 | −0.0570 | 0.207* | 0.25 (3) |
| H23E | 0.3773 | 0.6801 | −0.0238 | 0.207* | 0.25 (3) |
| H23F | 0.3339 | 0.6308 | 0.0597 | 0.207* | 0.25 (3) |
| N1 | 0.8600 (2) | 0.37943 (7) | 0.34558 (19) | 0.0484 (5) | |
| O1 | 0.9526 (2) | 0.29189 (7) | 0.42972 (19) | 0.0672 (6) | |
| O2 | 0.8019 (2) | 0.35559 (7) | 0.55794 (16) | 0.0678 (5) | |
| O3 | 0.5734 (3) | 0.55723 (9) | 0.5029 (2) | 0.0778 (6) | |
| O5 | 0.6935 (3) | 0.64938 (7) | 0.2993 (2) | 0.0852 (7) | |

| | | | | |
|---|---|---|---|---|
| S1 | 0.82591 (8) | 0.32957 (2) | 0.44398 (6) | 0.0503 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0451 (14) | 0.0345 (12) | 0.0580 (15) | 0.0042 (11) | −0.0034 (12) | 0.0042 (11) |
| C2 | 0.0622 (18) | 0.0516 (15) | 0.0561 (16) | −0.0040 (13) | −0.0039 (13) | 0.0003 (12) |
| C3 | 0.083 (2) | 0.0685 (19) | 0.077 (2) | −0.0151 (18) | −0.0250 (18) | −0.0036 (16) |
| C4 | 0.062 (2) | 0.073 (2) | 0.151 (4) | −0.0129 (18) | −0.035 (2) | 0.005 (2) |
| C5 | 0.049 (2) | 0.079 (2) | 0.171 (4) | 0.0067 (18) | 0.009 (2) | −0.003 (3) |
| C6 | 0.0562 (19) | 0.0530 (16) | 0.105 (2) | 0.0061 (14) | 0.0061 (17) | −0.0103 (16) |
| C7 | 0.0529 (15) | 0.0371 (12) | 0.0533 (15) | 0.0003 (11) | 0.0010 (12) | −0.0034 (11) |
| C8 | 0.0440 (14) | 0.0376 (12) | 0.0546 (15) | −0.0014 (11) | 0.0003 (11) | −0.0006 (11) |
| C9 | 0.0478 (15) | 0.0429 (13) | 0.0549 (15) | −0.0076 (11) | 0.0051 (12) | −0.0045 (11) |
| C10 | 0.078 (2) | 0.0557 (16) | 0.0657 (19) | −0.0134 (15) | 0.0154 (16) | −0.0019 (14) |
| C11 | 0.100 (3) | 0.079 (2) | 0.076 (2) | −0.016 (2) | 0.0355 (19) | −0.0140 (18) |
| C12 | 0.086 (2) | 0.064 (2) | 0.093 (3) | −0.0013 (17) | 0.036 (2) | −0.0192 (18) |
| C13 | 0.0634 (19) | 0.0469 (15) | 0.089 (2) | 0.0050 (14) | 0.0201 (16) | −0.0047 (14) |
| C14 | 0.0420 (14) | 0.0398 (13) | 0.0640 (17) | −0.0027 (11) | 0.0070 (12) | −0.0047 (11) |
| C15 | 0.0556 (16) | 0.0413 (13) | 0.0543 (15) | −0.0008 (11) | −0.0018 (12) | 0.0085 (11) |
| C16 | 0.0479 (14) | 0.0352 (12) | 0.0601 (16) | −0.0023 (11) | 0.0053 (12) | 0.0058 (11) |
| C17 | 0.0507 (15) | 0.0410 (13) | 0.0667 (17) | −0.0065 (11) | −0.0003 (13) | −0.0009 (11) |
| C18 | 0.0604 (19) | 0.0555 (16) | 0.0604 (18) | −0.0053 (14) | 0.0010 (15) | −0.0051 (13) |
| O4 | 0.077 (3) | 0.180 (7) | 0.056 (3) | −0.019 (4) | −0.006 (2) | −0.001 (4) |
| C19 | 0.125 (4) | 0.269 (9) | 0.063 (3) | −0.051 (6) | 0.014 (3) | 0.008 (4) |
| C20 | 0.125 (4) | 0.269 (9) | 0.063 (3) | −0.051 (6) | 0.014 (3) | 0.008 (4) |
| O4A | 0.068 (5) | 0.082 (6) | 0.048 (4) | −0.018 (5) | −0.002 (3) | −0.003 (4) |
| C19A | 0.125 (4) | 0.269 (9) | 0.063 (3) | −0.051 (6) | 0.014 (3) | 0.008 (4) |
| C20A | 0.125 (4) | 0.269 (9) | 0.063 (3) | −0.051 (6) | 0.014 (3) | 0.008 (4) |
| C21 | 0.0659 (19) | 0.0443 (15) | 0.0691 (19) | 0.0003 (13) | 0.0066 (16) | 0.0096 (14) |
| O6 | 0.086 (5) | 0.047 (4) | 0.094 (5) | 0.010 (4) | −0.018 (3) | 0.017 (4) |
| C22 | 0.118 (10) | 0.065 (4) | 0.148 (9) | 0.027 (8) | −0.043 (8) | 0.031 (5) |
| C23 | 0.097 (7) | 0.127 (7) | 0.160 (9) | −0.017 (7) | −0.056 (7) | 0.073 (7) |
| O6A | 0.11 (3) | 0.078 (18) | 0.095 (17) | 0.055 (14) | −0.047 (17) | −0.023 (13) |
| C22A | 0.054 (11) | 0.060 (12) | 0.119 (15) | 0.028 (11) | 0.013 (12) | 0.021 (9) |
| C23A | 0.071 (17) | 0.107 (18) | 0.23 (4) | 0.021 (18) | −0.03 (2) | 0.02 (2) |
| N1 | 0.0516 (12) | 0.0369 (10) | 0.0567 (13) | 0.0023 (9) | 0.0038 (10) | 0.0013 (9) |
| O1 | 0.0516 (11) | 0.0501 (10) | 0.0993 (15) | 0.0089 (9) | −0.0161 (10) | 0.0131 (10) |
| O2 | 0.0949 (15) | 0.0554 (11) | 0.0524 (9) | −0.0092 (10) | −0.0127 (10) | −0.0002 (8) |
| O3 | 0.0607 (14) | 0.0908 (15) | 0.0824 (15) | 0.0018 (12) | 0.0100 (11) | −0.0054 (11) |
| O5 | 0.125 (2) | 0.0359 (10) | 0.0949 (16) | 0.0041 (11) | 0.0001 (14) | −0.0016 (10) |
| S1 | 0.0524 (4) | 0.0392 (3) | 0.0587 (4) | −0.0003 (3) | −0.0119 (3) | 0.0059 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.366 (4) | C18—O4 | 1.323 (7) |
| C1—C2 | 1.386 (3) | C18—O4A | 1.380 (12) |
| C1—S1 | 1.748 (2) | O4—C19 | 1.456 (10) |

| | | | |
|---|---|---|---|
| C2—C3 | 1.379 (4) | C19—C20 | 1.507 (8) |
| C2—H2 | 0.9300 | C19—H19A | 0.9700 |
| C3—C4 | 1.355 (5) | C19—H19B | 0.9700 |
| C3—H3 | 0.9300 | C20—H20A | 0.9600 |
| C4—C5 | 1.375 (5) | C20—H20B | 0.9600 |
| C4—H4 | 0.9300 | C20—H20C | 0.9600 |
| C5—C6 | 1.380 (4) | O4A—C19A | 1.45 (2) |
| C5—H5 | 0.9300 | C19A—C20A | 1.485 (10) |
| C6—H6 | 0.9300 | C19A—H19C | 0.9700 |
| C7—C8 | 1.352 (3) | C19A—H19D | 0.9700 |
| C7—N1 | 1.392 (3) | C20A—H20D | 0.9600 |
| C7—H7 | 0.9300 | C20A—H20E | 0.9600 |
| C8—C9 | 1.439 (3) | C20A—H20F | 0.9600 |
| C8—C15 | 1.460 (3) | C21—O5 | 1.189 (3) |
| C9—C14 | 1.389 (3) | C21—O6 | 1.313 (17) |
| C9—C10 | 1.391 (4) | C21—O6A | 1.36 (5) |
| C10—C11 | 1.369 (4) | O6—C22 | 1.52 (2) |
| C10—H10 | 0.9300 | C22—C23 | 1.479 (8) |
| C11—C12 | 1.382 (5) | C22—H22A | 0.9700 |
| C11—H11 | 0.9300 | C22—H22B | 0.9700 |
| C12—C13 | 1.372 (4) | C23—H23A | 0.9600 |
| C12—H12 | 0.9300 | C23—H23B | 0.9600 |
| C13—C14 | 1.385 (3) | C23—H23C | 0.9600 |
| C13—H13 | 0.9300 | O6A—C22A | 1.51 (6) |
| C14—N1 | 1.408 (3) | C22A—C23A | 1.516 (10) |
| C15—C16 | 1.321 (3) | C22A—H22C | 0.9700 |
| C15—H15 | 0.9300 | C22A—H22D | 0.9700 |
| C16—C21 | 1.487 (3) | C23A—H23D | 0.9600 |
| C16—C17 | 1.494 (3) | C23A—H23E | 0.9600 |
| C17—C18 | 1.492 (4) | C23A—H23F | 0.9600 |
| C17—H17A | 0.9700 | N1—S1 | 1.663 (2) |
| C17—H17B | 0.9700 | O1—S1 | 1.4185 (18) |
| C18—O3 | 1.185 (3) | O2—S1 | 1.4202 (19) |
| | | | |
| C6—C1—C2 | 121.6 (3) | O4—C18—C17 | 109.2 (4) |
| C6—C1—S1 | 119.2 (2) | O4A—C18—C17 | 110.0 (6) |
| C2—C1—S1 | 119.2 (2) | C18—O4—C19 | 115.5 (6) |
| C3—C2—C1 | 118.5 (3) | O4—C19—C20 | 104.9 (7) |
| C3—C2—H2 | 120.8 | O4—C19—H19A | 110.8 |
| C1—C2—H2 | 120.8 | C20—C19—H19A | 110.8 |
| C4—C3—C2 | 120.3 (3) | O4—C19—H19B | 110.8 |
| C4—C3—H3 | 119.8 | C20—C19—H19B | 110.8 |
| C2—C3—H3 | 119.8 | H19A—C19—H19B | 108.8 |
| C3—C4—C5 | 120.9 (3) | C18—O4A—C19A | 117.9 (13) |
| C3—C4—H4 | 119.5 | O4A—C19A—C20A | 117.0 (14) |
| C5—C4—H4 | 119.5 | O4A—C19A—H19C | 108.1 |
| C4—C5—C6 | 119.9 (3) | C20A—C19A—H19C | 108.1 |
| C4—C5—H5 | 120.1 | O4A—C19A—H19D | 108.1 |

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|---|---|---|---|
| C6—C5—H5 | 120.1 | C20A—C19A—H19D | 108.1 |
| C1—C6—C5 | 118.8 (3) | H19C—C19A—H19D | 107.3 |
| C1—C6—H6 | 120.6 | C19A—C20A—H20D | 109.5 |
| C5—C6—H6 | 120.6 | C19A—C20A—H20E | 109.5 |
| C8—C7—N1 | 110.1 (2) | H20D—C20A—H20E | 109.5 |
| C8—C7—H7 | 125.0 | C19A—C20A—H20F | 109.5 |
| N1—C7—H7 | 125.0 | H20D—C20A—H20F | 109.5 |
| C7—C8—C9 | 106.9 (2) | H20E—C20A—H20F | 109.5 |
| C7—C8—C15 | 128.0 (2) | O5—C21—O6 | 124.1 (7) |
| C9—C8—C15 | 125.1 (2) | O5—C21—O6A | 121 (2) |
| C14—C9—C10 | 119.3 (2) | O5—C21—C16 | 123.9 (3) |
| C14—C9—C8 | 108.0 (2) | O6—C21—C16 | 111.9 (7) |
| C10—C9—C8 | 132.7 (2) | O6A—C21—C16 | 114 (2) |
| C11—C10—C9 | 118.5 (3) | C21—O6—C22 | 114.6 (13) |
| C11—C10—H10 | 120.7 | C23—C22—O6 | 102.5 (13) |
| C9—C10—H10 | 120.7 | C23—C22—H22A | 111.2 |
| C10—C11—C12 | 121.2 (3) | O6—C22—H22A | 111.3 |
| C10—C11—H11 | 119.4 | C23—C22—H22B | 111.2 |
| C12—C11—H11 | 119.4 | O6—C22—H22B | 111.3 |
| C13—C12—C11 | 121.7 (3) | H22A—C22—H22B | 109.2 |
| C13—C12—H12 | 119.2 | C21—O6A—C22A | 107 (3) |
| C11—C12—H12 | 119.2 | O6A—C22A—C23A | 98 (4) |
| C12—C13—C14 | 116.9 (3) | O6A—C22A—H22C | 112.3 |
| C12—C13—H13 | 121.6 | C23A—C22A—H22C | 112.1 |
| C14—C13—H13 | 121.6 | O6A—C22A—H22D | 111.9 |
| C13—C14—C9 | 122.4 (3) | C23A—C22A—H22D | 112.2 |
| C13—C14—N1 | 130.5 (2) | H22C—C22A—H22D | 109.8 |
| C9—C14—N1 | 107.1 (2) | C22A—C23A—H23D | 109.5 |
| C16—C15—C8 | 127.8 (2) | C22A—C23A—H23E | 109.5 |
| C16—C15—H15 | 116.1 | H23D—C23A—H23E | 109.5 |
| C8—C15—H15 | 116.1 | C22A—C23A—H23F | 109.5 |
| C15—C16—C21 | 121.6 (2) | H23D—C23A—H23F | 109.5 |
| C15—C16—C17 | 123.9 (2) | H23E—C23A—H23F | 109.5 |
| C21—C16—C17 | 114.5 (2) | C7—N1—C14 | 107.80 (19) |
| C18—C17—C16 | 113.0 (2) | C7—N1—S1 | 123.13 (18) |
| C18—C17—H17A | 109.0 | C14—N1—S1 | 126.13 (16) |
| C16—C17—H17A | 109.0 | O1—S1—O2 | 120.72 (12) |
| C18—C17—H17B | 109.0 | O1—S1—N1 | 106.02 (11) |
| C16—C17—H17B | 109.0 | O2—S1—N1 | 105.29 (10) |
| H17A—C17—H17B | 107.8 | O1—S1—C1 | 109.09 (11) |
| O3—C18—O4 | 124.1 (4) | O2—S1—C1 | 109.70 (13) |
| O3—C18—O4A | 119.9 (6) | N1—S1—C1 | 104.75 (11) |
| O3—C18—C17 | 125.8 (3) | | |

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|---|---|---|---|
| C6—C1—C2—C3 | 0.2 (4) | C18—O4—C19—C20 | 104.0 (8) |
| S1—C1—C2—C3 | −179.2 (2) | O3—C18—O4A—C19A | −11.3 (11) |
| C1—C2—C3—C4 | −0.2 (4) | O4—C18—O4A—C19A | 96.2 (17) |
| C2—C3—C4—C5 | −0.7 (5) | C17—C18—O4A—C19A | −169.3 (9) |

| | | | |
|---|---|---|---|
| C3—C4—C5—C6 | 1.6 (6) | C18—O4A—C19A—C20A | −97.2 (18) |
| C2—C1—C6—C5 | 0.6 (4) | C15—C16—C21—O5 | −172.0 (3) |
| S1—C1—C6—C5 | −179.9 (3) | C17—C16—C21—O5 | 7.1 (4) |
| C4—C5—C6—C1 | −1.5 (5) | C15—C16—C21—O6 | 3.4 (9) |
| N1—C7—C8—C9 | 2.2 (3) | C17—C16—C21—O6 | −177.5 (8) |
| N1—C7—C8—C15 | 179.5 (2) | C15—C16—C21—O6A | 19 (3) |
| C7—C8—C9—C14 | −1.2 (3) | C17—C16—C21—O6A | −162 (3) |
| C15—C8—C9—C14 | −178.7 (2) | O5—C21—O6—C22 | −15.6 (18) |
| C7—C8—C9—C10 | 179.4 (3) | O6A—C21—O6—C22 | 68 (10) |
| C15—C8—C9—C10 | 1.9 (4) | C16—C21—O6—C22 | 169.0 (11) |
| C14—C9—C10—C11 | 1.2 (4) | C21—O6—C22—C23 | 160.5 (12) |
| C8—C9—C10—C11 | −179.5 (3) | O5—C21—O6A—C22A | 37 (5) |
| C9—C10—C11—C12 | −1.2 (5) | O6—C21—O6A—C22A | −68 (9) |
| C10—C11—C12—C13 | 0.2 (5) | C16—C21—O6A—C22A | −154 (3) |
| C11—C12—C13—C14 | 0.8 (5) | C21—O6A—C22A—C23A | −167 (3) |
| C12—C13—C14—C9 | −0.8 (4) | C8—C7—N1—C14 | −2.3 (3) |
| C12—C13—C14—N1 | 179.9 (3) | C8—C7—N1—S1 | −163.95 (17) |
| C10—C9—C14—C13 | −0.1 (4) | C13—C14—N1—C7 | −179.1 (3) |
| C8—C9—C14—C13 | −179.6 (2) | C9—C14—N1—C7 | 1.5 (3) |
| C10—C9—C14—N1 | 179.3 (2) | C13—C14—N1—S1 | −18.2 (4) |
| C8—C9—C14—N1 | −0.2 (3) | C9—C14—N1—S1 | 162.42 (17) |
| C7—C8—C15—C16 | 41.3 (4) | C7—N1—S1—O1 | −161.85 (19) |
| C9—C8—C15—C16 | −141.8 (3) | C14—N1—S1—O1 | 39.9 (2) |
| C8—C15—C16—C21 | −176.4 (2) | C7—N1—S1—O2 | −32.8 (2) |
| C8—C15—C16—C17 | 4.6 (4) | C14—N1—S1—O2 | 169.0 (2) |
| C15—C16—C17—C18 | −99.6 (3) | C7—N1—S1—C1 | 82.8 (2) |
| C21—C16—C17—C18 | 81.3 (3) | C14—N1—S1—C1 | −75.4 (2) |
| C16—C17—C18—O3 | −15.0 (4) | C6—C1—S1—O1 | 149.7 (2) |
| C16—C17—C18—O4 | 175.7 (4) | C2—C1—S1—O1 | −30.8 (2) |
| C16—C17—C18—O4A | 141.5 (4) | C6—C1—S1—O2 | 15.5 (2) |
| O3—C18—O4—C19 | 10.8 (9) | C2—C1—S1—O2 | −165.07 (19) |
| O4A—C18—O4—C19 | −82.3 (14) | C6—C1—S1—N1 | −97.1 (2) |
| C17—C18—O4—C19 | −179.6 (6) | C2—C1—S1—N1 | 82.3 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13···O1 | 0.93 | 2.44 | 3.012 (4) | 120 |
| C12—H12···*Cg*2$^{i}$ | 0.93 | 2.80 | 3.561 (4) | 140 |

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