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# Ethyl 3-[2-benzyl-1-(phenylsulfonyl)-1*H*-indol-3-yl]acrylate

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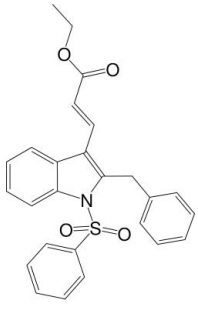
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.048; $wR$ factor = 0.119; data-to-parameter ratio = 27.4.

In the title compound, $C_{26}H_{23}NO_4S$, the planes of the ethyl acrylate group, the sulfonyl-bound phenyl ring and the benzyl phenyl group are inclined at angles of 7.91 (4), 81.39 (4) and 88.33 (4)°, respectively, with respect to the indole ring system. The conformations of the phenylsulfonyl and benzyl substituents with respect to the indole ring system are influenced by intramolecular C—H···O and C—H···$\pi$ interactions. Inversion-related molecules at ($x$, $y$, $z$) and ($-x$, 1 − $y$, $-z$) are linked into a centrosymmetric dimer by C—H···O hydrogen bonds. The dimers are crosslinked through C—H···$\pi$ interactions, forming a two-dimensional network parallel to the $bc$ plane. Weak $\pi$–$\pi$ stacking interactions are present between the phenyl rings of the benzyl groups; the centroid-to-centroid distance between the rings is 3.8027 (9) Å and the perpendicular distance is 3.743 Å.

## Related literature

For general background and related structures, see: Senthil Kumar *et al.* (2006*a*,*b*,*c*,*d*).




## Experimental

### Crystal data

$C_{26}H_{23}NO_4S$
$M_r$ = 445.51
Monoclinic, $P2_1/c$
$a$ = 11.4683 (2) Å
$b$ = 8.8983 (1) Å
$c$ = 21.5088 (3) Å
$\beta$ = 99.406 (1)°
$V$ = 2165.43 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 100.0 (1) K
0.28 × 0.25 × 0.24 mm

### Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.912, $T_{max}$ = 0.958
47728 measured reflections
7943 independent reflections
5869 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.119
$S$ = 1.06
7943 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7···O2 | 0.95 | 2.36 | 2.9424 (17) | 119 |
| C15—H15$A$···O1 | 0.99 | 2.24 | 2.8474 (17) | 118 |
| C18—H18···O3$^{i}$ | 0.95 | 2.59 | 3.282 (2) | 130 |
| C10—H10···$Cg1$ | 0.95 | 2.75 | 3.3524 (14) | 122 |
| C11—H11···$Cg2^{ii}$ | 0.95 | 2.81 | 3.6263 (15) | 145 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2193).

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# supplementary materials

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# Ethyl 3-[2-benzyl-1-(phenylsulfonyl)-1*H*-indol-3-yl]acrylate

**K. Chinnakali, R. Surendran, R. Balamurugan, A. K. Mohanakrishnan and H.-K. Fun**

## Comment

The background to this study is set out in Senthil Kumar *et al.* (2006*a*,b,c,d). We now describe the X-ray crystal structure determination of the title compound.

Bond distances and angles in the title compound are comparable to those observed for ethyl 3-(2-methoxycarbonylmethyl-1-phenylsulfonyl-1*H*-indol-3-yl)acrylate (Senthil Kumar *et al.*, 2006*c*). The indole ring system is planar with atom C5 deviating by a maximum of 0.027 (1) Å, from the mean plane through that ring system. As observed in other phenylsulfonylindoles (Senthil Kumar *et al.*, 2006*a*,b,c,d), atom S1 has a distorted tetrahedral configuration, with angles O1—S1—O2 [120.60 (6)°] and N1—S1—C9 [104.87 (6)°] deviating significantly from ideal tetrahedral values. The conformation of the phenylsulfonyl group with respect to the indole unit is described by the torsion angles O1—S1—N1—C1 = 22.55 (12)°, O2—S1—N1—C8 = −36.63 (11)° and N1—S1—C9—C10 = 98.91 (11)°. This conformation is influenced by the intramolecular C—H···O interactions, C7—H7···O2 and C15—H15A···O1, involving the sulfonyl O1 and O2 atoms which deviate 0.143 (1) and 0.509 (1) Å, respectively, from the plane of the indole ring system.

The dihedral angle between the C9—C14 phenyl ring and indole ring system is 81.39 (4)°. The torsion angle N1—C1—C15—C16 of 81.74 (15)° describes the conformation of the attachment of the benzyl substituent to the indole ring system and torsion angle C1—C15—C16—C21 of 24.17 (18)° shows how the C16—C21 phenyl ring is oriented. This conformation is influenced by the intramolecular C15—H15A···O1 interaction, and by the C—H···π interaction involving H10 and the C16—C21 ring, with H10 separated from the ring centroid (*Cg*1) by 2.75 Å (Table 1). The dihedral angle between the mean planes through the C9—C14 and C16—C21 aromatic rings is 33.35 (6)°; the centroids of these two rings are separated by 4.4737 (8) Å and hence there is no π-π interaction between them.

Atoms O3, O4, C22 to C26 of the ethyl acrylate substituent group at C2 are coplanar (r.m.s deviation of 0.054 Å). This plane is slightly twisted away from the indole ring system by an angle of 7.91 (4)°.

The C18—H18···O3 hydrogen bonds link the inversion-related molecules at (*x*, *y*, *z*) and (−*x*, 1 − *y*, −*z*) into a centrosymmetric dimer. The dimer structure is further stabilized by a weak π-π stacking interaction between the phenyl rings (C16—C21) of the benzyl groups; the centroid–centroid distance between the rings is 3.8027 (9) Å and the perpendicular distance is 3.743 Å. The dimers are linked through C—H···π interactions (Table 1) involving H11 and the benzene ring (C3—C8; centroid *Cg*2) of the indole ring system, to form a two-dimensional network parallel to the *bc* plane (Fig. 2).

## Experimental

(*E*)-Ethyl 3-[2-(hydroxymethyl)-1-(phenylsulfonyl)-1*H*-indol-3-yl)acrylate (1.3 mmol) and boron trifluoride etherate solution (5 drops) in dry benzene (20 ml) were refuxed for 4 h. After completion of the reaction, the mixture was poured into ice-water, washed with water (3 × 10 ml) followed by solvent removal to give the crude product. It was recrystallized from methanol (5 ml).

### Refinement

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.95 Å (C$sp^2$), 0.98 Å (methyl) and 0.99 Å (methylene), and $U_{iso}$(H) value of 1.2$U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$)

### Figures

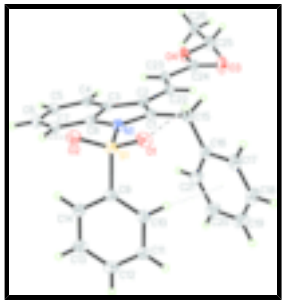

Fig. 1. Molecular structure of the title compound, showing the atomic numbering and 50% probability displacement ellipsoids. C—H···O hydrogen bonds are shown as dashed lines and the dotted line represents a C—H···π interaction.

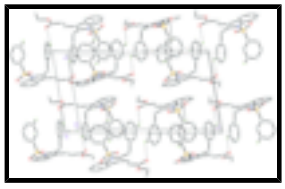

Fig. 2. Part of the crystal packing of the title compound, viewed approximately down the *b* axis. C—H···O hydrogen bonds are shown as dashed lines, C—H···π interactions are shown as double dashed lines and π–π interactions are shown as dotted lines. H atoms not involved in these interactions have been omitted.

### Ethyl 3-[2-benzyl-1-(phenylsulfonyl)-1*H*-indol-3-yl]acrylate

*Crystal data*

| | |
|---|---|
| $C_{26}H_{23}NO_4S$ | $F_{000}$ = 936 |
| $M_r$ = 445.51 | $D_x$ = 1.367 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 7382 reflections |
| $a$ = 11.4683 (2) Å | θ = 2.4–30.6º |
| $b$ = 8.8983 (1) Å | μ = 0.18 mm$^{-1}$ |
| $c$ = 21.5088 (3) Å | $T$ = 100.0 (1) K |
| β = 99.406 (1)º | Block, yellow |
| $V$ = 2165.43 (5) Å$^3$ | 0.28 × 0.25 × 0.24 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX2 CCD area-detector diffractometer | 7943 independent reflections |
| Radiation source: fine-focus sealed tube | 5869 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.060 |
| Detector resolution: 8.33 pixels mm$^{-1}$ | $\theta_{max}$ = 32.7º |
| $T$ = 100.0(1) K | $\theta_{min}$ = 1.9º |

| | |
|---|---|
| ω scans | $h = -17 \rightarrow 14$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | $k = -12 \rightarrow 13$ |
| $T_{min} = 0.912$, $T_{max} = 0.958$ | $l = -32 \rightarrow 31$ |
| 47728 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H-atom parameters constrained |
| $wR(F^2) = 0.119$ | $w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.737P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 7943 reflections | $\Delta\rho_{max} = 0.41$ e Å$^{-3}$ |
| 290 parameters | $\Delta\rho_{min} = -0.54$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2$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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.27475 (3) | 0.34607 (4) | 0.252973 (15) | 0.01888 (8) |
| O1 | 0.26409 (9) | 0.23974 (11) | 0.20278 (5) | 0.0246 (2) |
| O2 | 0.35867 (8) | 0.32365 (11) | 0.30905 (5) | 0.0235 (2) |
| O3 | 0.29725 (11) | 0.91913 (13) | −0.02392 (5) | 0.0337 (3) |
| O4 | 0.37486 (9) | 1.13030 (11) | 0.02295 (4) | 0.0255 (2) |
| N1 | 0.31080 (9) | 0.51204 (12) | 0.22307 (5) | 0.0177 (2) |
| C1 | 0.29109 (11) | 0.55791 (14) | 0.15938 (6) | 0.0173 (2) |
| C2 | 0.32209 (11) | 0.70722 (14) | 0.15648 (6) | 0.0168 (2) |
| C3 | 0.36031 (10) | 0.75975 (14) | 0.22039 (6) | 0.0164 (2) |
| C4 | 0.39607 (11) | 0.90026 (15) | 0.24600 (6) | 0.0181 (2) |
| H4 | 0.4010 | 0.9843 | 0.2193 | 0.022* |
| C5 | 0.42414 (12) | 0.91474 (16) | 0.31074 (6) | 0.0214 (3) |

| | | | | |
|---|---|---|---|---|
| H5 | 0.4468 | 1.0101 | 0.3286 | 0.026* |
| C6 | 0.41952 (12) | 0.79078 (16) | 0.35020 (6) | 0.0223 (3) |
| H6 | 0.4410 | 0.8029 | 0.3945 | 0.027* |
| C7 | 0.38426 (11) | 0.65075 (15) | 0.32612 (6) | 0.0203 (2) |
| H7 | 0.3812 | 0.5667 | 0.3530 | 0.024* |
| C8 | 0.35341 (11) | 0.63749 (14) | 0.26097 (6) | 0.0169 (2) |
| C9 | 0.13509 (11) | 0.37614 (14) | 0.27434 (6) | 0.0190 (2) |
| C10 | 0.03426 (12) | 0.32885 (16) | 0.23390 (6) | 0.0231 (3) |
| H10 | 0.0407 | 0.2792 | 0.1955 | 0.028* |
| C11 | −0.07581 (12) | 0.35557 (17) | 0.25069 (7) | 0.0261 (3) |
| H11 | −0.1455 | 0.3244 | 0.2236 | 0.031* |
| C12 | −0.08422 (12) | 0.42756 (16) | 0.30685 (7) | 0.0253 (3) |
| H12 | −0.1598 | 0.4472 | 0.3177 | 0.030* |
| C13 | 0.01697 (12) | 0.47128 (16) | 0.34750 (7) | 0.0250 (3) |
| H13 | 0.0102 | 0.5183 | 0.3864 | 0.030* |
| C14 | 0.12761 (12) | 0.44652 (15) | 0.33152 (6) | 0.0221 (3) |
| H14 | 0.1971 | 0.4769 | 0.3590 | 0.027* |
| C15 | 0.24417 (12) | 0.45820 (15) | 0.10488 (6) | 0.0206 (3) |
| H15A | 0.2807 | 0.3576 | 0.1124 | 0.025* |
| H15B | 0.2691 | 0.4996 | 0.0664 | 0.025* |
| C16 | 0.11042 (12) | 0.43986 (15) | 0.09285 (6) | 0.0206 (3) |
| C17 | 0.06111 (14) | 0.31429 (17) | 0.06005 (7) | 0.0265 (3) |
| H17 | 0.1112 | 0.2417 | 0.0456 | 0.032* |
| C18 | −0.06059 (14) | 0.29404 (18) | 0.04830 (7) | 0.0319 (3) |
| H18 | −0.0932 | 0.2079 | 0.0258 | 0.038* |
| C19 | −0.13458 (14) | 0.39880 (19) | 0.06916 (7) | 0.0317 (3) |
| H19 | −0.2177 | 0.3838 | 0.0617 | 0.038* |
| C20 | −0.08669 (13) | 0.52580 (19) | 0.10099 (7) | 0.0305 (3) |
| H20 | −0.1371 | 0.5985 | 0.1151 | 0.037* |
| C21 | 0.03539 (13) | 0.54664 (16) | 0.11225 (7) | 0.0253 (3) |
| H21 | 0.0677 | 0.6347 | 0.1334 | 0.030* |
| C22 | 0.31486 (11) | 0.78830 (15) | 0.09784 (6) | 0.0190 (2) |
| H22 | 0.2829 | 0.7339 | 0.0610 | 0.023* |
| C23 | 0.34727 (12) | 0.93034 (15) | 0.08850 (6) | 0.0213 (3) |
| H23 | 0.3773 | 0.9928 | 0.1233 | 0.026* |
| C24 | 0.33564 (12) | 0.98804 (15) | 0.02363 (6) | 0.0208 (3) |
| C25 | 0.36841 (14) | 1.19570 (17) | −0.03932 (6) | 0.0275 (3) |
| H25A | 0.2849 | 1.2104 | −0.0590 | 0.033* |
| H25B | 0.4067 | 1.1286 | −0.0667 | 0.033* |
| C26 | 0.43137 (16) | 1.34387 (17) | −0.03127 (7) | 0.0312 (3) |
| H26A | 0.4278 | 1.3922 | −0.0725 | 0.047* |
| H26B | 0.5141 | 1.3276 | −0.0124 | 0.047* |
| H26C | 0.3933 | 1.4087 | −0.0037 | 0.047* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.02132 (15) | 0.01453 (14) | 0.02155 (15) | 0.00192 (11) | 0.00570 (12) | 0.00244 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0317 (5) | 0.0159 (4) | 0.0278 (5) | 0.0009 (4) | 0.0100 (4) | −0.0008 (4) |
| O2 | 0.0225 (5) | 0.0228 (5) | 0.0251 (5) | 0.0049 (4) | 0.0039 (4) | 0.0079 (4) |
| O3 | 0.0488 (7) | 0.0312 (6) | 0.0189 (5) | −0.0167 (5) | −0.0013 (4) | 0.0008 (4) |
| O4 | 0.0393 (6) | 0.0207 (5) | 0.0161 (4) | −0.0072 (4) | 0.0032 (4) | 0.0031 (4) |
| N1 | 0.0201 (5) | 0.0155 (5) | 0.0175 (5) | −0.0005 (4) | 0.0036 (4) | 0.0012 (4) |
| C1 | 0.0178 (5) | 0.0181 (6) | 0.0166 (5) | 0.0000 (4) | 0.0044 (4) | −0.0004 (4) |
| C2 | 0.0165 (5) | 0.0170 (5) | 0.0171 (5) | −0.0005 (4) | 0.0032 (4) | 0.0004 (4) |
| C3 | 0.0144 (5) | 0.0178 (5) | 0.0170 (5) | 0.0007 (4) | 0.0025 (4) | 0.0004 (4) |
| C4 | 0.0178 (5) | 0.0178 (6) | 0.0189 (6) | −0.0006 (4) | 0.0034 (4) | −0.0006 (5) |
| C5 | 0.0213 (6) | 0.0222 (6) | 0.0200 (6) | −0.0027 (5) | 0.0020 (5) | −0.0031 (5) |
| C6 | 0.0224 (6) | 0.0272 (7) | 0.0163 (6) | −0.0009 (5) | 0.0000 (5) | −0.0008 (5) |
| C7 | 0.0203 (6) | 0.0227 (6) | 0.0174 (6) | 0.0008 (5) | 0.0012 (5) | 0.0032 (5) |
| C8 | 0.0150 (5) | 0.0169 (6) | 0.0189 (6) | 0.0007 (4) | 0.0030 (4) | 0.0003 (4) |
| C9 | 0.0199 (6) | 0.0171 (6) | 0.0209 (6) | −0.0002 (4) | 0.0055 (5) | 0.0033 (5) |
| C10 | 0.0255 (6) | 0.0238 (6) | 0.0201 (6) | −0.0054 (5) | 0.0044 (5) | 0.0004 (5) |
| C11 | 0.0211 (6) | 0.0310 (7) | 0.0258 (7) | −0.0063 (5) | 0.0025 (5) | 0.0024 (6) |
| C12 | 0.0219 (6) | 0.0227 (6) | 0.0324 (7) | −0.0008 (5) | 0.0075 (5) | 0.0036 (6) |
| C13 | 0.0255 (7) | 0.0231 (6) | 0.0278 (7) | −0.0008 (5) | 0.0087 (5) | −0.0037 (5) |
| C14 | 0.0218 (6) | 0.0219 (6) | 0.0226 (6) | −0.0013 (5) | 0.0033 (5) | −0.0015 (5) |
| C15 | 0.0258 (6) | 0.0176 (6) | 0.0186 (6) | −0.0026 (5) | 0.0047 (5) | −0.0025 (5) |
| C16 | 0.0242 (6) | 0.0197 (6) | 0.0173 (6) | −0.0038 (5) | 0.0015 (5) | 0.0015 (5) |
| C17 | 0.0327 (7) | 0.0235 (7) | 0.0222 (6) | −0.0042 (6) | 0.0006 (5) | −0.0026 (5) |
| C18 | 0.0353 (8) | 0.0285 (7) | 0.0284 (7) | −0.0109 (6) | −0.0052 (6) | 0.0019 (6) |
| C19 | 0.0244 (7) | 0.0380 (8) | 0.0299 (8) | −0.0064 (6) | −0.0037 (6) | 0.0095 (7) |
| C20 | 0.0252 (7) | 0.0334 (8) | 0.0317 (8) | 0.0019 (6) | 0.0009 (6) | 0.0039 (6) |
| C21 | 0.0256 (7) | 0.0227 (7) | 0.0269 (7) | −0.0018 (5) | 0.0017 (5) | −0.0013 (5) |
| C22 | 0.0194 (6) | 0.0205 (6) | 0.0170 (5) | −0.0018 (5) | 0.0025 (4) | 0.0001 (5) |
| C23 | 0.0261 (6) | 0.0214 (6) | 0.0157 (6) | −0.0035 (5) | 0.0013 (5) | 0.0005 (5) |
| C24 | 0.0221 (6) | 0.0219 (6) | 0.0180 (6) | −0.0032 (5) | 0.0024 (5) | 0.0019 (5) |
| C25 | 0.0378 (8) | 0.0271 (7) | 0.0171 (6) | −0.0044 (6) | 0.0030 (5) | 0.0067 (5) |
| C26 | 0.0492 (9) | 0.0227 (7) | 0.0239 (7) | −0.0045 (6) | 0.0121 (7) | 0.0036 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4257 (10) | C12—C13 | 1.389 (2) |
| S1—O2 | 1.4288 (10) | C12—H12 | 0.95 |
| S1—N1 | 1.6889 (11) | C13—C14 | 1.3853 (19) |
| S1—C9 | 1.7574 (13) | C13—H13 | 0.95 |
| O3—C24 | 1.2118 (16) | C14—H14 | 0.95 |
| O4—C24 | 1.3443 (16) | C15—C16 | 1.5220 (19) |
| O4—C25 | 1.4510 (16) | C15—H15A | 0.99 |
| N1—C1 | 1.4118 (16) | C15—H15B | 0.99 |
| N1—C8 | 1.4210 (16) | C16—C21 | 1.391 (2) |
| C1—C2 | 1.3794 (18) | C16—C17 | 1.3913 (19) |
| C1—C15 | 1.4984 (17) | C17—C18 | 1.389 (2) |
| C2—C22 | 1.4436 (18) | C17—H17 | 0.95 |
| C2—C3 | 1.4503 (17) | C18—C19 | 1.384 (2) |
| C3—C4 | 1.4004 (18) | C18—H18 | 0.95 |
| C3—C8 | 1.4051 (17) | C19—C20 | 1.387 (2) |

| | | | |
|---|---|---|---|
| C4—C5 | 1.3830 (18) | C19—H19 | 0.95 |
| C4—H4 | 0.95 | C20—C21 | 1.394 (2) |
| C5—C6 | 1.3980 (19) | C20—H20 | 0.95 |
| C5—H5 | 0.95 | C21—H21 | 0.95 |
| C6—C7 | 1.3842 (19) | C22—C23 | 1.3418 (18) |
| C6—H6 | 0.95 | C22—H22 | 0.95 |
| C7—C8 | 1.3930 (18) | C23—C24 | 1.4722 (18) |
| C7—H7 | 0.95 | C23—H23 | 0.95 |
| C9—C10 | 1.3935 (19) | C25—C26 | 1.500 (2) |
| C9—C14 | 1.3954 (19) | C25—H25A | 0.99 |
| C10—C11 | 1.389 (2) | C25—H25B | 0.99 |
| C10—H10 | 0.95 | C26—H26A | 0.98 |
| C11—C12 | 1.384 (2) | C26—H26B | 0.98 |
| C11—H11 | 0.95 | C26—H26C | 0.98 |
| O1—S1—O2 | 120.60 (6) | C13—C14—C9 | 118.74 (12) |
| O1—S1—N1 | 106.74 (6) | C13—C14—H14 | 120.6 |
| O2—S1—N1 | 105.69 (6) | C9—C14—H14 | 120.6 |
| O1—S1—C9 | 109.27 (6) | C1—C15—C16 | 114.81 (11) |
| O2—S1—C9 | 108.51 (6) | C1—C15—H15A | 108.6 |
| N1—S1—C9 | 104.87 (6) | C16—C15—H15A | 108.6 |
| C24—O4—C25 | 114.90 (11) | C1—C15—H15B | 108.6 |
| C1—N1—C8 | 108.36 (10) | C16—C15—H15B | 108.6 |
| C1—N1—S1 | 127.73 (9) | H15A—C15—H15B | 107.5 |
| C8—N1—S1 | 123.44 (9) | C21—C16—C17 | 118.73 (13) |
| C2—C1—N1 | 108.71 (11) | C21—C16—C15 | 122.10 (12) |
| C2—C1—C15 | 126.67 (11) | C17—C16—C15 | 119.15 (12) |
| N1—C1—C15 | 124.62 (11) | C18—C17—C16 | 120.63 (15) |
| C1—C2—C22 | 122.85 (12) | C18—C17—H17 | 119.7 |
| C1—C2—C3 | 107.92 (11) | C16—C17—H17 | 119.7 |
| C22—C2—C3 | 129.23 (12) | C19—C18—C17 | 120.32 (14) |
| C4—C3—C8 | 119.31 (11) | C19—C18—H18 | 119.8 |
| C4—C3—C2 | 133.18 (12) | C17—C18—H18 | 119.8 |
| C8—C3—C2 | 107.48 (11) | C18—C19—C20 | 119.64 (14) |
| C5—C4—C3 | 118.96 (12) | C18—C19—H19 | 120.2 |
| C5—C4—H4 | 120.5 | C20—C19—H19 | 120.2 |
| C3—C4—H4 | 120.5 | C19—C20—C21 | 119.97 (15) |
| C4—C5—C6 | 120.81 (12) | C19—C20—H20 | 120.0 |
| C4—C5—H5 | 119.6 | C21—C20—H20 | 120.0 |
| C6—C5—H5 | 119.6 | C16—C21—C20 | 120.67 (14) |
| C7—C6—C5 | 121.38 (12) | C16—C21—H21 | 119.7 |
| C7—C6—H6 | 119.3 | C20—C21—H21 | 119.7 |
| C5—C6—H6 | 119.3 | C23—C22—C2 | 128.59 (12) |
| C6—C7—C8 | 117.60 (12) | C23—C22—H22 | 115.7 |
| C6—C7—H7 | 121.2 | C2—C22—H22 | 115.7 |
| C8—C7—H7 | 121.2 | C22—C23—C24 | 119.08 (12) |
| C7—C8—C3 | 121.90 (12) | C22—C23—H23 | 120.5 |
| C7—C8—N1 | 130.59 (12) | C24—C23—H23 | 120.5 |
| C3—C8—N1 | 107.51 (11) | O3—C24—O4 | 122.91 (12) |
| C10—C9—C14 | 121.43 (12) | O3—C24—C23 | 125.98 (13) |

| | | | |
|---|---|---|---|
| C10—C9—S1 | 119.31 (10) | O4—C24—C23 | 111.10 (11) |
| C14—C9—S1 | 119.26 (10) | O4—C25—C26 | 107.16 (12) |
| C11—C10—C9 | 118.86 (13) | O4—C25—H25A | 110.3 |
| C11—C10—H10 | 120.6 | C26—C25—H25A | 110.3 |
| C9—C10—H10 | 120.6 | O4—C25—H25B | 110.3 |
| C12—C11—C10 | 120.13 (13) | C26—C25—H25B | 110.3 |
| C12—C11—H11 | 119.9 | H25A—C25—H25B | 108.5 |
| C10—C11—H11 | 119.9 | C25—C26—H26A | 109.5 |
| C11—C12—C13 | 120.56 (13) | C25—C26—H26B | 109.5 |
| C11—C12—H12 | 119.7 | H26A—C26—H26B | 109.5 |
| C13—C12—H12 | 119.7 | C25—C26—H26C | 109.5 |
| C14—C13—C12 | 120.27 (13) | H26A—C26—H26C | 109.5 |
| C14—C13—H13 | 119.9 | H26B—C26—H26C | 109.5 |
| C12—C13—H13 | 119.9 | | |
| O1—S1—N1—C1 | 22.55 (12) | O2—S1—C9—C10 | −148.51 (11) |
| O2—S1—N1—C1 | 152.10 (11) | N1—S1—C9—C10 | 98.91 (11) |
| C9—S1—N1—C1 | −93.33 (11) | O1—S1—C9—C14 | 164.62 (10) |
| O1—S1—N1—C8 | −166.17 (10) | O2—S1—C9—C14 | 31.32 (12) |
| O2—S1—N1—C8 | −36.63 (11) | N1—S1—C9—C14 | −81.26 (11) |
| C9—S1—N1—C8 | 77.95 (11) | C14—C9—C10—C11 | 1.3 (2) |
| C8—N1—C1—C2 | 1.03 (14) | S1—C9—C10—C11 | −178.86 (11) |
| S1—N1—C1—C2 | 173.37 (9) | C9—C10—C11—C12 | −0.2 (2) |
| C8—N1—C1—C15 | −178.99 (11) | C10—C11—C12—C13 | −1.2 (2) |
| S1—N1—C1—C15 | −6.66 (18) | C11—C12—C13—C14 | 1.6 (2) |
| N1—C1—C2—C22 | 178.70 (11) | C12—C13—C14—C9 | −0.5 (2) |
| C15—C1—C2—C22 | −1.3 (2) | C10—C9—C14—C13 | −1.0 (2) |
| N1—C1—C2—C3 | −1.33 (14) | S1—C9—C14—C13 | 179.21 (11) |
| C15—C1—C2—C3 | 178.70 (12) | C2—C1—C15—C16 | −98.29 (15) |
| C1—C2—C3—C4 | −176.70 (13) | N1—C1—C15—C16 | 81.74 (15) |
| C22—C2—C3—C4 | 3.3 (2) | C1—C15—C16—C21 | 24.17 (18) |
| C1—C2—C3—C8 | 1.14 (14) | C1—C15—C16—C17 | −157.46 (12) |
| C22—C2—C3—C8 | −178.89 (12) | C21—C16—C17—C18 | −1.6 (2) |
| C8—C3—C4—C5 | 0.24 (18) | C15—C16—C17—C18 | 179.96 (13) |
| C2—C3—C4—C5 | 177.87 (13) | C16—C17—C18—C19 | 0.0 (2) |
| C3—C4—C5—C6 | 1.37 (19) | C17—C18—C19—C20 | 1.1 (2) |
| C4—C5—C6—C7 | −1.5 (2) | C18—C19—C20—C21 | −0.5 (2) |
| C5—C6—C7—C8 | 0.0 (2) | C17—C16—C21—C20 | 2.2 (2) |
| C6—C7—C8—C3 | 1.65 (19) | C15—C16—C21—C20 | −179.43 (13) |
| C6—C7—C8—N1 | −177.70 (12) | C19—C20—C21—C16 | −1.1 (2) |
| C4—C3—C8—C7 | −1.79 (18) | C1—C2—C22—C23 | −176.57 (13) |
| C2—C3—C8—C7 | −179.98 (11) | C3—C2—C22—C23 | 3.5 (2) |
| C4—C3—C8—N1 | 177.69 (11) | C2—C22—C23—C24 | 177.74 (13) |
| C2—C3—C8—N1 | −0.50 (13) | C25—O4—C24—O3 | −0.3 (2) |
| C1—N1—C8—C7 | 179.12 (13) | C25—O4—C24—C23 | 179.10 (12) |
| S1—N1—C8—C7 | 6.38 (19) | C22—C23—C24—O3 | 1.0 (2) |
| C1—N1—C8—C3 | −0.31 (13) | C22—C23—C24—O4 | −178.39 (12) |
| S1—N1—C8—C3 | −173.04 (8) | C24—O4—C25—C26 | −171.93 (13) |
| O1—S1—C9—C10 | −15.21 (13) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···O2 | 0.95 | 2.36 | 2.9424 (17) | 119 |
| C15—H15A···O1 | 0.99 | 2.24 | 2.8474 (17) | 118 |
| C18—H18···O3$^{i}$ | 0.95 | 2.59 | 3.282 (2) | 130 |
| C10—H10···Cg1 | 0.95 | 2.75 | 3.3524 (14) | 122 |
| C11—H11···Cg2$^{ii}$ | 0.95 | 2.81 | 3.6263 (15) | 145 |

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

**Fig. 1**

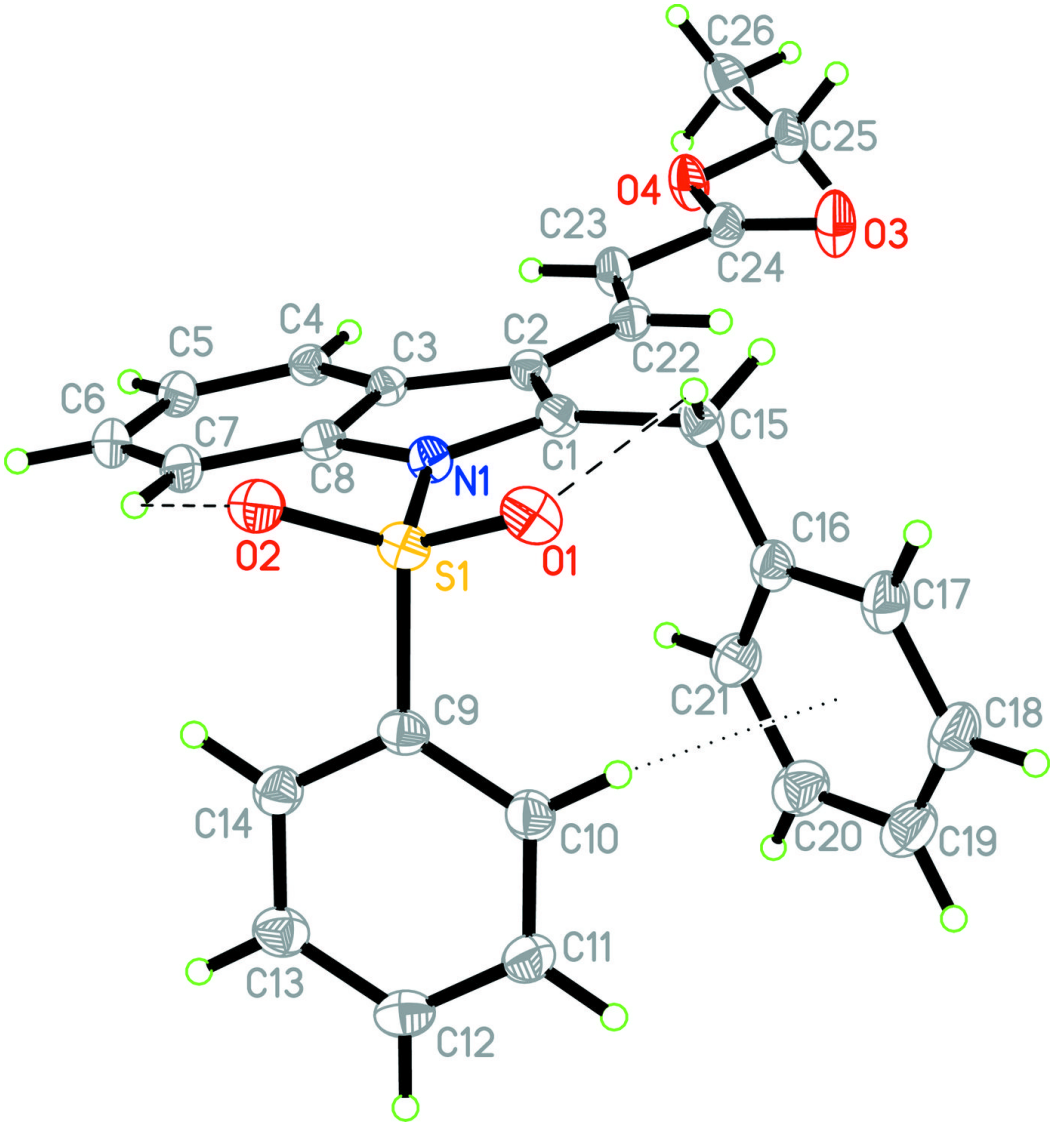
C26
C25
O4
O3
C23
C24
C4
C5
C3
C2
C22
C6
C7
C8
N1
C1
C15
O2
S1
O1
C16
C17
C21
C18
C9
C14
C10
C20
C19
C11
C13
C12

**Fig. 2**