Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-3-Phenyl-2-(1-tosyl-1*H*-indol-3-ylcarbonyl)acrylonitrile

S. Paramasivam,[a] G. Bhaskar,[b] P. R. Seshadri[a]* and P. T. Perumal[b]

[a]Postgraduate and Research Department of Physics, Agurchand Manmull Jain College, Chennai 600 114, India, and [b]Organic Chemistry Division, Central Leather Research Institute, Chennai 600 020, India
Correspondence e-mail: seshadri_pr@yahoo.com

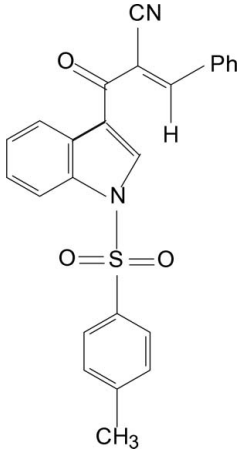
Received 27 January 2012; accepted 4 February 2012

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.176; data-to-parameter ratio = 18.8.

In the title compound, $C_{25}H_{18}N_2O_3S$, the indole moiety is planar and makes a dihedral angle of 89.95 (09)° with the phenyl ring of the sulfonyl substituent. The molecular conformation features a weak C—H···N short contact and the crystal packing reveals a weak C—H···O hydrogen bond.

Related literature

For the biological activity of indole derivatives, see: Andreani *et al.* (2001); Chai *et al.* (2006); Kolocouris *et al.* (1994); Ma *et al.* (2001); Nieto *et al.* (2005); Singh *et al.* (2000). For the bond-length difference, see: Allen (1981); Govindasamy *et al.* (1998); Sankaranarayanan *et al.* (2000). For the N atom-hybridization, see: Beddoes *et al.* (1986). For related structures, see: Seshadri *et al.* (2002).



Experimental

Crystal data

$C_{25}H_{18}N_2O_3S$
M_r = 426.47
Monoclinic, $C2/c$
a = 33.8741 (13) Å
b = 7.1294 (3) Å
c = 19.9180 (9) Å
β = 118.4170 (2)°
V = 4230.6 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 K
0.21 × 0.19 × 0.15 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
19948 measured reflections
5285 independent reflections
2177 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.176
S = 0.95
5285 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···N2	0.93	2.73	3.433 (4)	133
C5—H5···O3^{i}	0.93	2.86	3.551 (4)	132

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*, *PLATON* and *publCIF* (Westrip, 2010).

The authors acknowledge the Technology Business Incubator (TBI), CAS in Crystallography, University of Madras, Chennai, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2387).

References

Allen, F. H. (1981). *Acta Cryst.* B**37**, 900–906.
Andreani, A., Granaiola, M., Leoni, A., Locatelli, A., Morigi, R., Rambaldi, M., Giorgi, G., Salvini, L. & Garaliene, V. (2001). *Anti-Cancer Drug Des.* **16**, 167–174.
Beddoes, R. L., Dalton, L., Joule, T. A., Mills, O. S., Street, J. D. & Watt, C. I. F. (1986). *J. Chem. Soc. Perkin Trans. 2*, pp. 787–797.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Ins., Madison, Wisconsin, USA.
Chai, H., Zhao, C. & Gong, P. (2006). *Bioorg. Med. Chem.* **14**, 911–917.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Govindasamy, L., Velmurugan, D., Ravikumar, K. & Mohanakrishnan, A. K. (1998). *Acta Cryst.* C**54**, 277–279.
Kolocouris, N., Foscolos, G. B., Kolocouris, A., Marakos, P., Pouli, N., Fytas, G., Ikeda, S. & De Clercq, E. (1994). *J. Med. Chem.* **37**, 2896–2902.
Ma, C., Liu, X., Li, X., Flippen-Anderson, J., Yu, S. & Cook, J. M. (2001). *J. Org. Chem.* **66**, 4525–4542.
Nieto, M. J., Alovero, F. L., Manzo, R. H. & Mazzieri, M. R. (2005). *Eur. J. Med. Chem.* **40**, 361–369.
Sankaranarayanan, R., Velmurugan, D., Shanmuga Sundara Raj, S., Fun, H.-K., Babu, G. & Perumal, P. T. (2000). *Acta Cryst.* C**56**, 475–476.
Seshadri, P. R., Velmurugan, D., Govindaraj, J., Kannadasan, S., Srinivasan, P. C., Shanmuga Sundara Raj, S., Fun, H.-K. & Kim, M. J. (2002). *Acta Cryst.* C**58**, o700–o703.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Singh, U. P., Sarma, B. K., Mishra, P. K. & Ray, A. B. (2000). *Folia Microbiol. (Praha)*, **45**, 173–176.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2012). E**68**, o683–o684 [doi:10.1107/S1600536812004886]

(*E*)-3-Phenyl-2-(1-tosyl-1*H*-indol-3-ylcarbonyl)acrylonitrile

S. Paramasivam, G. Bhaskar, P. R. Seshadri and P. T. Perumal

Comment

Indole derivatives exhibit anti-bacterial (Nieto *et al.*, 2005), anti-cancer, anti-malarial and anti-hypertensive (Ma *et al.*, 2001) activities. In addition, indole derivatives are known to exhibit anti-fungal (Singh *et al.*, 2000), anti-tumour (Andreani *et al.*, 2001), anti-viral (Kolocouris *et al.*, 1994) and anti-hepatitis B virus (Chai *et al.*, 2006) activities. Against this background, the title compound was chosen for X-ray structure analysis (Fig.1).

The indole ring is planar and the sulfonyl bound phenyl ring is perpendicular to the nine membered indole moiety with a dihedral angle of 89.95 (09)°.

The torsion angles O1—S1—N1—C1 and O2—S1—N1—C7 [45.9 (3)° and -23.3 (3)°, respectively] indicates the syn conformation of the sulfonyl moiety. The sum of the bond angles around N1 [357.95 (23)°] indicates sp^2 hybridization (Beddoes *et al.*,1986).

A distorted tetrahedral geometry [O1—S1—O2 = 120.75 (13)° and O1—S1—N1 = 104.53 (12)°] around S1 is observed. The widening of the angles may be due to repulsive interactions between the two short S═O bonds.

In the benzene ring of the indole system, the *endo*-cyclic angles at C2, C5 and C6 are contracted to 116.9 (3)°, 118.6 (3)° and 118.5 (3)° respectively, while those at C1, C3 and C4 expanded to 123.3 (3)°, 121.5 (3)° and 121.2 (3)° respectively. This may be due to a real effect caused by the fusion of the smaller pyrrole ring to the six membered benzene ring, and the strain is taken up by angular distortion rather than by bond length distortions (Allen, 1981). A similar effect has also been observed by Sankaranarayanan *et al.* (2000) and Seshadri *et al.* (2002).

The difference in C—N bond lengths may be due to the electron-withdrawing character of the phenyl sulfonyl group (Govindasamy *et al.*, 1998; Seshadri *et al.*, 2002). The molecular structure is stabilised by a weak C—H···N intramolecular interactions and the crystal packing reveals a weak C—H···O hydrogen bond.

Experimental

To the mixture of cyanoacetylindole(2 mmol) and benzaldehyde (2.1 mmol) sodium methoxide (10 mol %) was added in methanol. The mixture was allowed to reflux for 2 h. After completion of the reaction, which was washed with water and extracted with ethylacetate (10 × 2 = 20 ml), the filtrate was dried with sodium sulfate and concentrated. The crude was subjected to column chromatography to obtain pure condensed chalcone product. To the chalcone (1 mmol) which was suspended in 10 ml benzene add aqueous 30% NaOH (10 ml), containing tosyl chloride (1.1 mmol) and tetrabutyl-ammonium bromide (0.10 mmol). After stirring vigorously for 30 min, the layers were separated and the water layer was extracted with benzene (10 ml). The combined organic layers were dried over Na_2SO_4 and the solvent was removed under reduced pressure. The crude product was purified by recrystallisation from CH_2Cl_2/hexane to afford (*E*)-3-phenyl-2-(1-tosyl-1*H*-indole-3-carbonyl)acrylonitrile.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2 U_{eq}(C) for other H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

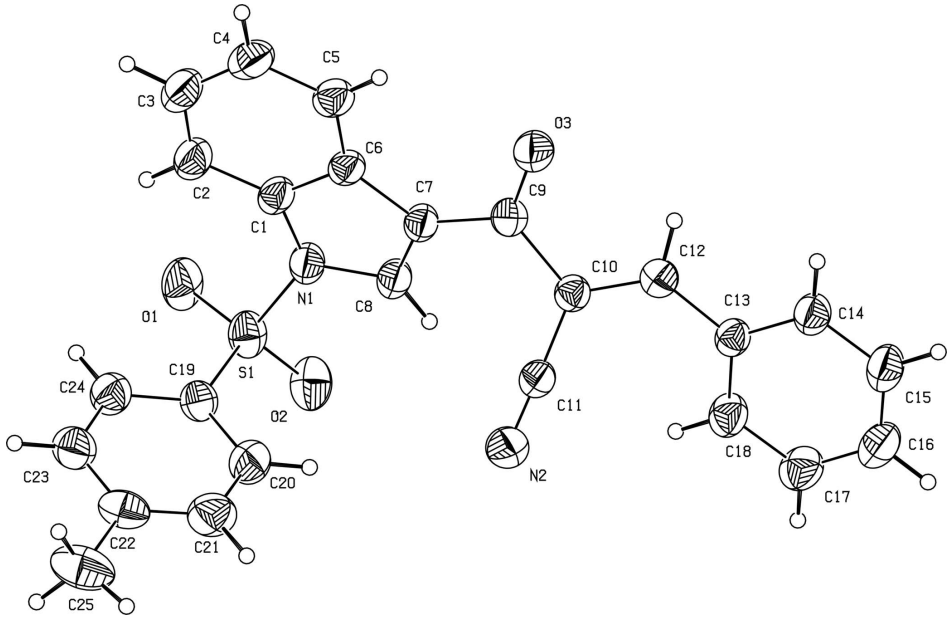


Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

(*E*)-3-Phenyl-2-(1-tosyl-1*H*-indol-3-ylcarbonyl)acrylonitrile

Crystal data

$C_{25}H_{18}N_2O_3S$
M_r = 426.47
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 33.8741 (13) Å
b = 7.1294 (3) Å
c = 19.9180 (9) Å
β = 118.4170 (2)°
V = 4230.6 (3) Å^3
Z = 8

F(000) = 1776
D_x = 1.339 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5285 reflections
θ = 1.4–28.4°
μ = 0.18 mm^{-1}
T = 298 K
Block, colourless
0.21 × 0.19 × 0.15 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
19948 measured reflections
5285 independent reflections
2177 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.4°$
$h = -44 \rightarrow 45$
$k = -9 \rightarrow 9$
$l = -26 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.176$
$S = 0.95$
5285 reflections
281 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
$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

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 $F^2 > \sigma(F^2)$ 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	0.31518 (8)	0.3247 (4)	0.26078 (18)	0.0600 (7)
C2	0.30356 (10)	0.4960 (4)	0.2794 (2)	0.0746 (9)
H2	0.3167	0.5385	0.3296	0.090*
C3	0.27188 (11)	0.5994 (4)	0.2206 (3)	0.0848 (10)
H3	0.2632	0.7148	0.2310	0.102*
C4	0.25246 (10)	0.5359 (4)	0.1457 (2)	0.0800 (9)
H4	0.2306	0.6085	0.1071	0.096*
C5	0.26497 (9)	0.3665 (4)	0.12750 (19)	0.0699 (8)
H5	0.2521	0.3259	0.0771	0.084*
C6	0.29717 (8)	0.2582 (4)	0.18621 (17)	0.0564 (7)
C7	0.31823 (8)	0.0804 (4)	0.18886 (16)	0.0555 (7)
C8	0.34654 (9)	0.0440 (4)	0.26354 (16)	0.0592 (7)
H8	0.3643	−0.0626	0.2817	0.071*
C9	0.30954 (9)	−0.0416 (4)	0.12459 (16)	0.0591 (7)
C10	0.34231 (8)	−0.1964 (4)	0.13431 (14)	0.0536 (7)
C11	0.38775 (10)	−0.1755 (4)	0.19112 (16)	0.0576 (7)
C12	0.32800 (9)	−0.3435 (4)	0.08643 (15)	0.0578 (7)
H12	0.2983	−0.3363	0.0482	0.069*

C13	0.35158 (9)	−0.5115 (4)	0.08504 (15)	0.0546 (7)
C14	0.33458 (9)	−0.6116 (4)	0.01750 (17)	0.0658 (8)
H14	0.3087	−0.5700	−0.0248	0.079*
C15	0.35560 (11)	−0.7728 (4)	0.0120 (2)	0.0774 (9)
H15	0.3440	−0.8379	−0.0339	0.093*
C16	0.39340 (11)	−0.8362 (4)	0.0741 (2)	0.0812 (9)
H16	0.4079	−0.9431	0.0700	0.097*
C17	0.41011 (11)	−0.7421 (4)	0.1426 (2)	0.0809 (9)
H17	0.4353	−0.7876	0.1852	0.097*
C18	0.38943 (10)	−0.5804 (4)	0.14814 (17)	0.0713 (8)
H18	0.4009	−0.5170	0.1945	0.086*
C19	0.42361 (9)	0.3581 (4)	0.39664 (15)	0.0606 (7)
C20	0.45161 (10)	0.2880 (5)	0.37005 (18)	0.0793 (9)
H20	0.4490	0.1638	0.3541	0.095*
C21	0.48304 (11)	0.4022 (6)	0.36733 (19)	0.0887 (10)
H21	0.5017	0.3542	0.3493	0.106*
C22	0.48793 (10)	0.5860 (5)	0.39046 (18)	0.0789 (10)
C23	0.45972 (10)	0.6538 (5)	0.41689 (19)	0.0803 (9)
H23	0.4625	0.7779	0.4329	0.096*
C24	0.42765 (10)	0.5417 (4)	0.42011 (17)	0.0716 (8)
H24	0.4089	0.5896	0.4380	0.086*
C25	0.52268 (11)	0.7124 (6)	0.3866 (2)	0.1128 (13)
H25A	0.5393	0.6429	0.3672	0.169*
H25B	0.5428	0.7582	0.4368	0.169*
H25C	0.5080	0.8164	0.3534	0.169*
N1	0.34515 (7)	0.1880 (3)	0.30873 (13)	0.0630 (6)
N2	0.42442 (9)	−0.1524 (3)	0.23564 (16)	0.0792 (8)
O1	0.36234 (7)	0.3040 (3)	0.43741 (12)	0.0896 (7)
O2	0.40187 (7)	0.0271 (3)	0.42345 (11)	0.0830 (6)
O3	0.27557 (7)	−0.0232 (3)	0.06329 (12)	0.0832 (6)
S1	0.38381 (3)	0.21122 (11)	0.40061 (4)	0.0698 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0581 (16)	0.0485 (17)	0.088 (2)	−0.0027 (14)	0.0464 (16)	−0.0045 (16)
C2	0.0714 (19)	0.064 (2)	0.105 (2)	−0.0046 (17)	0.0555 (19)	−0.0165 (19)
C3	0.079 (2)	0.058 (2)	0.142 (3)	−0.0015 (18)	0.072 (2)	−0.009 (2)
C4	0.0670 (19)	0.060 (2)	0.120 (3)	0.0096 (16)	0.051 (2)	0.013 (2)
C5	0.0605 (17)	0.0593 (19)	0.096 (2)	0.0004 (15)	0.0419 (17)	0.0019 (17)
C6	0.0508 (15)	0.0480 (16)	0.077 (2)	−0.0012 (13)	0.0361 (15)	0.0000 (15)
C7	0.0586 (16)	0.0462 (16)	0.0676 (18)	−0.0012 (13)	0.0347 (15)	−0.0047 (14)
C8	0.0658 (17)	0.0487 (16)	0.0690 (19)	0.0006 (13)	0.0370 (16)	−0.0050 (14)
C9	0.0588 (16)	0.0520 (17)	0.0646 (18)	−0.0011 (14)	0.0277 (15)	−0.0014 (14)
C10	0.0556 (15)	0.0493 (16)	0.0567 (16)	0.0007 (13)	0.0275 (14)	0.0008 (13)
C11	0.0592 (18)	0.0532 (17)	0.0608 (17)	0.0045 (14)	0.0288 (16)	−0.0009 (14)
C12	0.0603 (16)	0.0562 (17)	0.0595 (17)	−0.0012 (14)	0.0305 (14)	0.0026 (14)
C13	0.0584 (16)	0.0473 (16)	0.0651 (17)	−0.0017 (13)	0.0352 (14)	−0.0012 (14)
C14	0.0714 (18)	0.0610 (18)	0.0725 (19)	−0.0006 (15)	0.0403 (16)	−0.0085 (15)
C15	0.093 (2)	0.064 (2)	0.090 (2)	−0.0005 (18)	0.055 (2)	−0.0148 (18)

C16	0.090 (2)	0.059 (2)	0.117 (3)	0.0085 (18)	0.067 (2)	0.002 (2)
C17	0.082 (2)	0.060 (2)	0.099 (3)	0.0091 (17)	0.042 (2)	0.0116 (19)
C18	0.081 (2)	0.0520 (18)	0.080 (2)	0.0044 (16)	0.0374 (18)	0.0024 (15)
C19	0.0656 (17)	0.0619 (19)	0.0548 (16)	−0.0023 (15)	0.0290 (14)	−0.0033 (14)
C20	0.079 (2)	0.082 (2)	0.087 (2)	−0.0003 (18)	0.0478 (19)	−0.0138 (18)
C21	0.075 (2)	0.110 (3)	0.093 (2)	−0.002 (2)	0.050 (2)	−0.007 (2)
C22	0.0578 (18)	0.095 (3)	0.070 (2)	−0.0026 (18)	0.0193 (16)	0.0178 (19)
C23	0.072 (2)	0.065 (2)	0.089 (2)	−0.0021 (17)	0.0269 (18)	0.0049 (17)
C24	0.0721 (19)	0.067 (2)	0.080 (2)	−0.0013 (16)	0.0406 (17)	−0.0026 (17)
C25	0.073 (2)	0.143 (4)	0.111 (3)	−0.020 (2)	0.034 (2)	0.029 (3)
N1	0.0689 (14)	0.0563 (14)	0.0699 (15)	−0.0030 (12)	0.0381 (13)	−0.0106 (13)
N2	0.0704 (17)	0.0706 (17)	0.0851 (18)	0.0043 (14)	0.0276 (15)	0.0005 (14)
O1	0.1087 (16)	0.0969 (17)	0.0961 (16)	−0.0169 (13)	0.0755 (14)	−0.0299 (13)
O2	0.1187 (17)	0.0612 (13)	0.0717 (13)	−0.0003 (12)	0.0473 (12)	0.0074 (10)
O3	0.0740 (13)	0.0767 (14)	0.0737 (13)	0.0158 (11)	0.0147 (12)	−0.0106 (11)
S1	0.0880 (6)	0.0691 (6)	0.0650 (5)	−0.0087 (4)	0.0467 (4)	−0.0094 (4)

Geometric parameters (Å, º)

C1—C2	1.386 (4)	C14—H14	0.9300
C1—C6	1.393 (4)	C15—C16	1.366 (4)
C1—N1	1.404 (3)	C15—H15	0.9300
C2—C3	1.368 (5)	C16—C17	1.378 (5)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.389 (5)	C17—C18	1.380 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.384 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C24	1.375 (4)
C5—C6	1.393 (4)	C19—C20	1.381 (4)
C5—H5	0.9300	C19—S1	1.738 (3)
C6—C7	1.443 (3)	C20—C21	1.362 (4)
C7—C8	1.357 (4)	C20—H20	0.9300
C7—C9	1.457 (4)	C21—C22	1.373 (5)
C8—N1	1.381 (3)	C21—H21	0.9300
C8—H8	0.9300	C22—C23	1.379 (4)
C9—O3	1.223 (3)	C22—C25	1.513 (4)
C9—C10	1.511 (3)	C23—C24	1.375 (4)
C10—C12	1.343 (3)	C23—H23	0.9300
C11—N2	1.144 (3)	C24—H24	0.9300
C11—N2	1.144 (3)	C25—H25A	0.9600
C12—C13	1.447 (4)	C25—H25B	0.9600
C12—H12	0.9300	C25—H25C	0.9600
C13—C14	1.383 (4)	N1—S1	1.676 (2)
C13—C18	1.390 (4)	O1—S1	1.418 (2)
C14—C15	1.383 (4)	O2—S1	1.428 (2)
C2—C1—C6	123.3 (3)	C14—C15—H15	120.0
C2—C1—N1	129.4 (3)	C15—C16—C17	120.1 (3)
C6—C1—N1	107.3 (2)	C15—C16—H16	120.0
C3—C2—C1	116.9 (3)	C17—C16—H16	120.0

C3—C2—H2	121.6	C16—C17—C18	120.1 (3)
C1—C2—H2	121.6	C16—C17—H17	120.0
C2—C3—C4	121.5 (3)	C18—C17—H17	120.0
C2—C3—H3	119.3	C17—C18—C13	120.5 (3)
C4—C3—H3	119.3	C17—C18—H18	119.7
C5—C4—C3	121.2 (3)	C13—C18—H18	119.7
C5—C4—H4	119.4	C24—C19—C20	120.0 (3)
C3—C4—H4	119.4	C24—C19—S1	120.8 (2)
C4—C5—C6	118.6 (3)	C20—C19—S1	119.2 (2)
C4—C5—H5	120.7	C21—C20—C19	119.4 (3)
C6—C5—H5	120.7	C21—C20—H20	120.3
C1—C6—C5	118.5 (3)	C19—C20—H20	120.3
C1—C6—C7	107.6 (2)	C20—C21—C22	122.0 (3)
C5—C6—C7	133.9 (3)	C20—C21—H21	119.0
C8—C7—C6	106.7 (2)	C22—C21—H21	119.0
C8—C7—C9	126.2 (2)	C21—C22—C23	117.9 (3)
C6—C7—C9	127.1 (3)	C21—C22—C25	121.6 (3)
C7—C8—N1	110.3 (2)	C23—C22—C25	120.5 (4)
C7—C8—H8	124.9	C24—C23—C22	121.4 (3)
N1—C8—H8	124.9	C24—C23—H23	119.3
O3—C9—C7	120.9 (2)	C22—C23—H23	119.3
O3—C9—C10	119.4 (2)	C23—C24—C19	119.4 (3)
C7—C9—C10	119.6 (2)	C23—C24—H24	120.3
C12—C10—C11	122.4 (2)	C19—C24—H24	120.3
C12—C10—C9	119.0 (2)	C22—C25—H25A	109.5
C11—C10—C9	118.5 (2)	C22—C25—H25B	109.5
N2—C11—C10	177.4 (3)	H25A—C25—H25B	109.5
N2—C11—C10	177.4 (3)	C22—C25—H25C	109.5
C10—C12—C13	130.1 (2)	H25A—C25—H25C	109.5
C10—C12—H12	115.0	H25B—C25—H25C	109.5
C13—C12—H12	115.0	C8—N1—C1	108.1 (2)
C14—C13—C18	118.4 (3)	C8—N1—S1	122.25 (19)
C14—C13—C12	117.9 (3)	C1—N1—S1	127.6 (2)
C18—C13—C12	123.7 (3)	O1—S1—O2	120.75 (13)
C15—C14—C13	120.9 (3)	O1—S1—N1	106.49 (12)
C15—C14—H14	119.5	O2—S1—N1	104.53 (12)
C13—C14—H14	119.5	O1—S1—C19	110.00 (14)
C16—C15—C14	120.0 (3)	O2—S1—C19	110.14 (13)
C16—C15—H15	120.0	N1—S1—C19	103.28 (12)

C6—C1—C2—C3	1.7 (4)	C14—C15—C16—C17	1.3 (5)
N1—C1—C2—C3	−177.8 (3)	C15—C16—C17—C18	−1.9 (5)
C1—C2—C3—C4	−0.3 (4)	C16—C17—C18—C13	0.3 (5)
C2—C3—C4—C5	−1.1 (5)	C14—C13—C18—C17	1.7 (4)
C3—C4—C5—C6	1.0 (4)	C12—C13—C18—C17	179.8 (2)
C2—C1—C6—C5	−1.8 (4)	S1—C19—C20—C21	−179.6 (2)
N1—C1—C6—C5	177.8 (2)	C19—C20—C21—C22	0.1 (5)
C2—C1—C6—C7	177.9 (2)	C20—C21—C22—C23	−0.1 (5)
N1—C1—C6—C7	−2.5 (3)	C20—C21—C22—C25	−179.5 (3)

C4—C5—C6—C1	0.4 (4)	C25—C22—C23—C24	179.3 (3)
C4—C5—C6—C7	−179.3 (3)	C22—C23—C24—C19	0.1 (5)
C1—C6—C7—C8	1.8 (3)	C20—C19—C24—C23	−0.1 (4)
C5—C6—C7—C8	−178.5 (3)	S1—C19—C24—C23	179.4 (2)
C1—C6—C7—C9	179.2 (2)	C7—C8—N1—C1	−1.1 (3)
C5—C6—C7—C9	−1.1 (5)	C7—C8—N1—S1	−166.10 (19)
C6—C7—C8—N1	−0.5 (3)	C2—C1—N1—C8	−178.2 (3)
C9—C7—C8—N1	−177.9 (2)	C6—C1—N1—C8	2.2 (3)
C8—C7—C9—O3	159.9 (3)	C2—C1—N1—S1	−14.2 (4)
C6—C7—C9—O3	−17.1 (4)	C6—C1—N1—S1	166.19 (18)
C8—C7—C9—C10	−18.5 (4)	C8—N1—S1—O1	−152.2 (2)
C6—C7—C9—C10	164.5 (2)	C1—N1—S1—O1	45.9 (2)
O3—C9—C10—C12	−20.6 (4)	C8—N1—S1—O2	−23.3 (2)
C7—C9—C10—C12	157.8 (2)	C1—N1—S1—O2	174.8 (2)
O3—C9—C10—C11	155.9 (3)	C8—N1—S1—C19	91.9 (2)
C7—C9—C10—C11	−25.7 (3)	C1—N1—S1—C19	−70.0 (2)
C11—C10—C12—C13	6.3 (4)	C24—C19—S1—O1	−6.2 (3)
C9—C10—C12—C13	−177.3 (2)	C20—C19—S1—O1	173.4 (2)
C10—C12—C13—C14	−159.8 (3)	C24—C19—S1—O2	−141.6 (2)
C10—C12—C13—C18	22.1 (4)	C20—C19—S1—O2	37.9 (3)
C18—C13—C14—C15	−2.2 (4)	C24—C19—S1—N1	107.2 (2)
C12—C13—C14—C15	179.6 (2)	C20—C19—S1—N1	−73.3 (2)
C13—C14—C15—C16	0.7 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···N2	0.93	2.73	3.433 (4)	133
C5—H5···O3^{i}	0.93	2.86	3.551 (4)	132

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