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(E)-2-Bromo-1-[2-(2-nitrophenyl)-1-phenylsulfonyl-1H-indol-3-yl]ethanoneJ. Kanchanadevi,^a G. Anbalagan,^b V. Saravanan,^c
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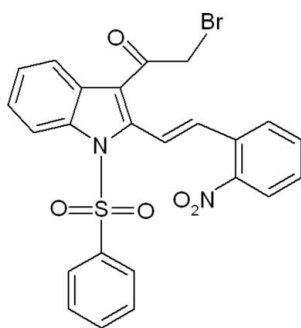
Received 5 January 2014; accepted 8 January 2014

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 14.5.

In the title compound $\text{C}_{24}\text{H}_{17}\text{BrN}_2\text{O}_5\text{S}$, the phenyl ring makes dihedral angles of 85.4 (2) and 8.8 (2)° with the indole ring system and the nitrobenzene ring, respectively, while the indole ring system and nitrobenzene ring make a dihedral angle of 80.1 (2)°. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ interactions link the molecules, forming a two-dimensional network parallel to the bc plane.

Related literature

For the biological activity of indole derivatives, see: Andreani *et al.* (2001); Singh *et al.* (2000); Pomarnacka & Kozlarska-Kedra (2003); Srivastava & Pandeya (2011). For a related structure, see: Umadevi *et al.* (2013); Kanchanadevi *et al.* (2013).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{17}\text{BrN}_2\text{O}_5\text{S}$
 $M_r = 525.37$
Monoclinic, Pn
 $a = 10.1823$ (7) Å
 $b = 8.0932$ (6) Å
 $c = 13.8111$ (12) Å
 $\beta = 102.749$ (2)°

$V = 1110.08$ (15) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.99$ mm⁻¹
 $T = 295$ K
 $0.35 \times 0.25 \times 0.25$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.543$, $T_{\max} = 0.609$

17011 measured reflections
4323 independent reflections
3368 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.116$
 $S = 1.01$
4323 reflections
298 parameters
2 restraints
H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.85$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³
Absolute structure: Flack (1983),
2093 Friedel pairs
Absolute structure parameter:
0.022 (9)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}5^i$	0.93	2.38	3.147 (5)	139

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

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: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5374).

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supplementary materials

Acta Cryst. (2014). E70, o149 [doi:10.1107/S1600536814000488]

(E)-2-Bromo-1-[2-(2-nitrostyryl)-1-phenylsulfonyl-1H-indol-3-yl]ethanone

J. Kanchanadevi, G. Anbalagan, V. Saravanan, A. K. Mohanakrishnan, B. Gunasekaran and V. Manivannan

1. Comment

Indole derivatives exhibits antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). These derivatives also exhibits antimicrobial, antibiotic, analgesic, anticancer and anti-HIV (Pomarnacka & Kozlarska-Kedra, 2003; Srivastava & Pandeya, 2011) activities.

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Umadevi *et al.*, 2013). The phenyl ring makes a dihedral angles of 85.4 (2)^o and 8.8 (2)^o with the indole ring system and the nitro benzene ring, respectively. The sum of bond angles around the atom N1 [355.7^o] indicates *sp*² hybridization. The molecular structure is stabilized by weak intramolecular C—H \cdots O interactions and the crystal packing is controlled by weak intermolecular C—H \cdots O interaction.

2. Experimental

A solution of 2-nitrophenylvinyl-3-acetylindole (1.0 g, 2.29 mmol) and PTT (Phenyl trimethyl ammonium tribromide) (0.92 g, 2.46 mmol) in dry THF (10 ml) was stirred at 10 ^o C for 1 h. After completion of the reaction (monitored by TLC), it was poured into crushed ice (100 g). The solid obtained was filtered and washed with MeOH (5 ml) to afford (E)-2-bromo-1-(2-(2-nitrostyryl)-1-(phenylsulfonyl)-1H-indol-3-yl)ethanone as a yellow solid (0.92 g, 78%) with melting point 184–186 ^o C.

3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C—H, C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); 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* (Sheldrick, 2008).

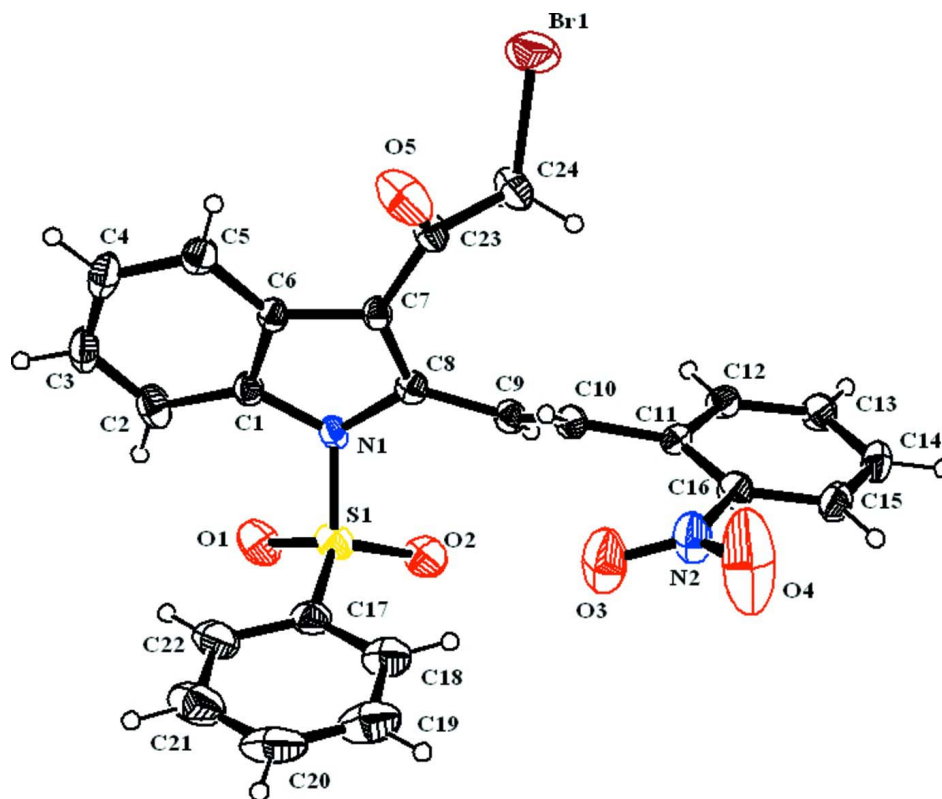
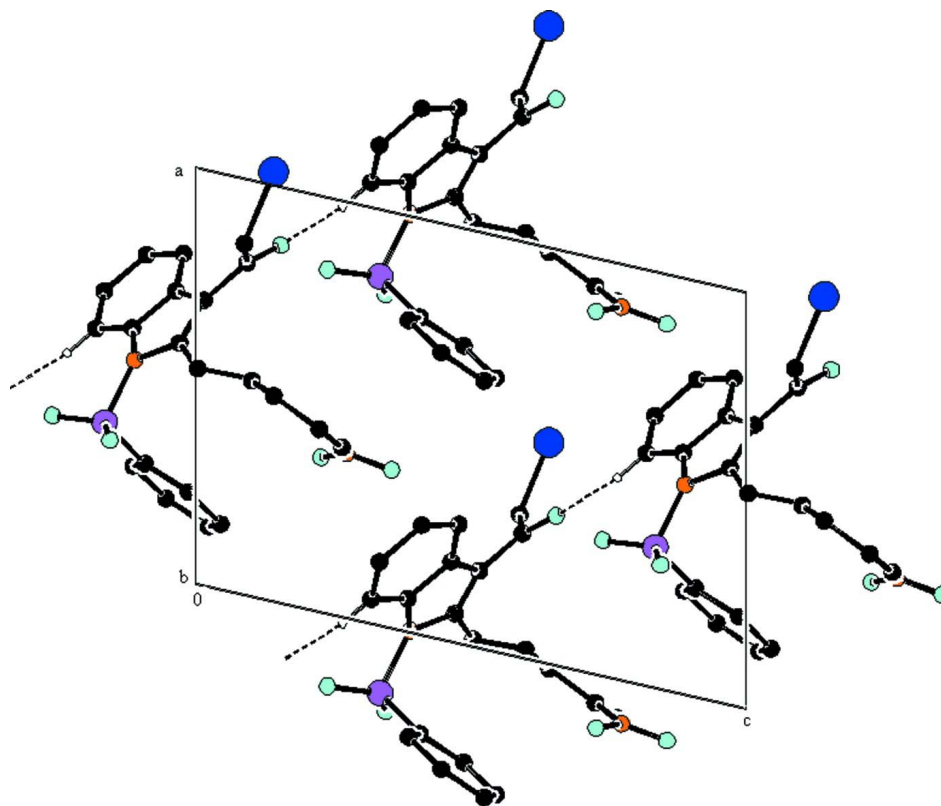


Figure 1

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

**Figure 2**

The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

(*E*)-2-Bromo-1-[2-(2-nitrostyryl)-1-phenylsulfonyl-1*H*-indol-3-yl]ethanone

Crystal data

$C_{24}H_{17}BrN_2O_5S$

$M_r = 525.37$

Monoclinic, *Pn*

Hall symbol: *P* -2*yac*

$a = 10.1823$ (7) Å

$b = 8.0932$ (6) Å

$c = 13.8111$ (12) Å

$\beta = 102.749$ (2)°

$V = 1110.08$ (15) Å³

$Z = 2$

$F(000) = 532$

$D_x = 1.572$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 4350 reflections

$\theta = 2.3$ – 26.3 °

$\mu = 1.99$ mm⁻¹

$T = 295$ K

Block, yellow

$0.35 \times 0.25 \times 0.25$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm⁻¹

ω and φ scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.543$, $T_{\max} = 0.609$

17011 measured reflections

4323 independent reflections

3368 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 26.3$ °, $\theta_{\min} = 2.3$ °

$h = -12 \rightarrow 12$

$k = -9 \rightarrow 9$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.116$

$S = 1.01$

4323 reflections

298 parameters

2 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

$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.3412P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack (1983), 2093 Friedel
pairs

Absolute structure parameter: 0.022 (9)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0805 (4)	0.3950 (5)	0.3857 (3)	0.0358 (8)
C2	0.0594 (5)	0.5284 (5)	0.3192 (3)	0.0516 (11)
H2	-0.0157	0.5329	0.2669	0.062*
C3	0.1535 (5)	0.6512 (5)	0.3345 (4)	0.0556 (11)
H3	0.1419	0.7411	0.2915	0.067*
C4	0.2643 (5)	0.6461 (5)	0.4112 (3)	0.0516 (11)
H4	0.3264	0.7319	0.4184	0.062*
C5	0.2867 (5)	0.5171 (5)	0.4783 (3)	0.0437 (10)
H5	0.3617	0.5156	0.5309	0.052*
C6	0.1926 (4)	0.3890 (4)	0.4643 (3)	0.0327 (8)
C7	0.1862 (4)	0.2356 (4)	0.5157 (3)	0.0307 (7)
C8	0.0699 (4)	0.1549 (4)	0.4711 (3)	0.0332 (8)
C9	0.0184 (4)	0.0034 (4)	0.5039 (3)	0.0353 (8)
H9	-0.0185	-0.0765	0.4574	0.042*
C10	0.0230 (4)	-0.0236 (4)	0.5997 (3)	0.0340 (8)
H10	0.0499	0.0638	0.6432	0.041*
C11	-0.0110 (3)	-0.1803 (5)	0.6424 (3)	0.0330 (8)
C12	0.0184 (4)	-0.3288 (4)	0.6024 (3)	0.0366 (9)
H12	0.0557	-0.3276	0.5467	0.044*
C13	-0.0058 (4)	-0.4776 (5)	0.6424 (3)	0.0445 (10)
H13	0.0152	-0.5753	0.6138	0.053*
C14	-0.0612 (5)	-0.4832 (5)	0.7250 (4)	0.0483 (11)
H14	-0.0772	-0.5844	0.7522	0.058*
C15	-0.0924 (4)	-0.3399 (5)	0.7662 (3)	0.0462 (10)
H15	-0.1307	-0.3427	0.8214	0.055*
C16	-0.0671 (4)	-0.1910 (5)	0.7261 (3)	0.0391 (9)
C17	-0.2379 (4)	0.3680 (6)	0.4081 (3)	0.0478 (11)
C18	-0.2824 (5)	0.3030 (7)	0.4874 (4)	0.0632 (13)
H18	-0.2719	0.1908	0.5016	0.076*
C19	-0.3424 (6)	0.4035 (10)	0.5456 (5)	0.0866 (19)
H19	-0.3735	0.3600	0.5987	0.104*
C20	-0.3552 (5)	0.5662 (10)	0.5243 (6)	0.088 (2)
H20	-0.3955	0.6344	0.5636	0.106*
C21	-0.3106 (6)	0.6341 (8)	0.4465 (6)	0.086 (2)

H21	-0.3205	0.7468	0.4339	0.103*
C22	-0.2511 (5)	0.5356 (6)	0.3871 (5)	0.0660 (14)
H22	-0.2204	0.5803	0.3341	0.079*
C23	0.2995 (4)	0.1765 (5)	0.5939 (3)	0.0380 (8)
C24	0.3438 (5)	-0.0005 (5)	0.5889 (4)	0.0540 (12)
H24A	0.3226	-0.0366	0.5203	0.065*
H24B	0.2936	-0.0696	0.6254	0.065*
N1	0.0045 (3)	0.2503 (4)	0.3896 (2)	0.0356 (7)
N2	-0.1036 (5)	-0.0428 (5)	0.7741 (3)	0.0598 (11)
O1	-0.1734 (3)	0.3120 (5)	0.2399 (2)	0.0654 (9)
O2	-0.2013 (3)	0.0745 (4)	0.3449 (2)	0.0602 (9)
O3	-0.1280 (5)	0.0831 (5)	0.7280 (4)	0.1015 (17)
O4	-0.1194 (10)	-0.0537 (6)	0.8566 (4)	0.171 (4)
O5	0.3599 (4)	0.2701 (4)	0.6549 (3)	0.0840 (13)
S1	-0.16138 (10)	0.24019 (13)	0.33528 (8)	0.0465 (3)
Br1	0.53169 (7)	-0.02967 (7)	0.64210 (6)	0.0930 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.041 (2)	0.0338 (19)	0.0347 (19)	0.0033 (16)	0.0131 (16)	0.0055 (16)
C2	0.068 (3)	0.046 (2)	0.041 (2)	0.009 (2)	0.012 (2)	0.0114 (19)
C3	0.078 (3)	0.035 (2)	0.063 (3)	0.005 (2)	0.035 (3)	0.015 (2)
C4	0.072 (3)	0.031 (2)	0.064 (3)	-0.0046 (19)	0.040 (3)	-0.0004 (19)
C5	0.048 (2)	0.039 (2)	0.050 (2)	0.0000 (17)	0.0229 (19)	-0.0033 (18)
C6	0.0388 (19)	0.0250 (18)	0.037 (2)	0.0017 (15)	0.0154 (16)	-0.0031 (16)
C7	0.0379 (19)	0.0241 (18)	0.0314 (18)	0.0009 (15)	0.0103 (15)	-0.0018 (14)
C8	0.0386 (19)	0.0281 (19)	0.0337 (18)	0.0002 (15)	0.0094 (15)	-0.0067 (15)
C9	0.038 (2)	0.028 (2)	0.039 (2)	-0.0018 (15)	0.0053 (16)	-0.0013 (15)
C10	0.0364 (19)	0.0233 (17)	0.043 (2)	0.0005 (15)	0.0108 (17)	-0.0048 (15)
C11	0.0287 (17)	0.033 (2)	0.038 (2)	-0.0034 (14)	0.0090 (16)	0.0015 (16)
C12	0.0358 (19)	0.033 (2)	0.044 (2)	0.0006 (16)	0.0136 (17)	-0.0053 (16)
C13	0.050 (3)	0.029 (2)	0.057 (3)	0.0020 (16)	0.017 (2)	-0.0053 (19)
C14	0.057 (3)	0.031 (2)	0.059 (3)	-0.0047 (18)	0.016 (2)	0.0098 (19)
C15	0.052 (2)	0.043 (2)	0.049 (2)	0.000 (2)	0.0239 (19)	0.008 (2)
C16	0.045 (2)	0.0307 (19)	0.044 (2)	0.0013 (17)	0.0143 (18)	-0.0052 (17)
C17	0.032 (2)	0.050 (3)	0.057 (3)	-0.0010 (17)	0.0001 (19)	-0.008 (2)
C18	0.052 (3)	0.069 (3)	0.069 (3)	0.001 (2)	0.015 (2)	-0.012 (3)
C19	0.059 (3)	0.102 (5)	0.105 (5)	-0.008 (3)	0.032 (3)	-0.036 (4)
C20	0.042 (3)	0.101 (6)	0.123 (6)	0.002 (3)	0.021 (3)	-0.049 (4)
C21	0.056 (3)	0.064 (4)	0.128 (6)	0.010 (3)	0.001 (4)	-0.033 (4)
C22	0.045 (3)	0.055 (3)	0.092 (4)	0.008 (2)	0.004 (3)	-0.009 (3)
C23	0.045 (2)	0.030 (2)	0.035 (2)	-0.0002 (17)	0.0018 (17)	-0.0032 (16)
C24	0.057 (3)	0.039 (2)	0.056 (3)	0.0065 (19)	-0.009 (2)	0.001 (2)
N1	0.0380 (16)	0.0322 (16)	0.0351 (16)	0.0039 (13)	0.0050 (13)	0.0071 (13)
N2	0.090 (3)	0.039 (2)	0.060 (3)	0.0112 (19)	0.038 (2)	-0.0005 (19)
O1	0.072 (2)	0.073 (2)	0.0417 (17)	0.0108 (18)	-0.0076 (15)	0.0061 (15)
O2	0.0532 (18)	0.0504 (19)	0.068 (2)	-0.0068 (14)	-0.0050 (16)	-0.0124 (15)
O3	0.160 (5)	0.047 (2)	0.127 (4)	0.025 (2)	0.097 (4)	0.008 (2)
O4	0.381 (12)	0.081 (3)	0.095 (4)	0.049 (5)	0.149 (6)	0.003 (3)

O5	0.090 (3)	0.051 (2)	0.084 (3)	0.0122 (18)	-0.037 (2)	-0.0277 (19)
S1	0.0421 (5)	0.0469 (6)	0.0439 (5)	0.0024 (5)	-0.0046 (4)	-0.0057 (5)
Br1	0.0538 (3)	0.0647 (3)	0.1580 (7)	0.0143 (3)	0.0183 (3)	-0.0032 (4)

Geometric parameters (Å, °)

C1—C6	1.392 (5)	C14—H14	0.9300
C1—C2	1.403 (6)	C15—C16	1.374 (6)
C1—N1	1.412 (5)	C15—H15	0.9300
C2—C3	1.364 (7)	C16—N2	1.457 (5)
C2—H2	0.9300	C17—C18	1.379 (7)
C3—C4	1.368 (7)	C17—C22	1.387 (7)
C3—H3	0.9300	C17—S1	1.742 (4)
C4—C5	1.381 (6)	C18—C19	1.378 (8)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.396 (6)	C19—C20	1.349 (11)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.439 (5)	C20—C21	1.370 (10)
C7—C8	1.373 (5)	C20—H20	0.9300
C7—C23	1.475 (5)	C21—C22	1.378 (8)
C8—N1	1.406 (5)	C21—H21	0.9300
C8—C9	1.445 (5)	C22—H22	0.9300
C9—C10	1.332 (5)	C23—O5	1.197 (5)
C9—H9	0.9300	C23—C24	1.508 (5)
C10—C11	1.472 (5)	C24—Br1	1.907 (5)
C10—H10	0.9300	C24—H24A	0.9700
C11—C12	1.383 (5)	C24—H24B	0.9700
C11—C16	1.400 (5)	N1—S1	1.692 (3)
C12—C13	1.370 (5)	N2—O4	1.188 (6)
C12—H12	0.9300	N2—O3	1.198 (5)
C13—C14	1.380 (6)	O1—S1	1.420 (3)
C13—H13	0.9300	O2—S1	1.416 (3)
C14—C15	1.361 (6)		
C6—C1—C2	121.2 (4)	C16—C15—H15	120.1
C6—C1—N1	107.7 (3)	C15—C16—C11	122.3 (3)
C2—C1—N1	131.1 (4)	C15—C16—N2	116.7 (4)
C3—C2—C1	117.3 (4)	C11—C16—N2	121.1 (3)
C3—C2—H2	121.3	C18—C17—C22	120.4 (5)
C1—C2—H2	121.3	C18—C17—S1	119.9 (4)
C2—C3—C4	121.9 (4)	C22—C17—S1	119.6 (4)
C2—C3—H3	119.0	C19—C18—C17	120.3 (6)
C4—C3—H3	119.0	C19—C18—H18	119.9
C3—C4—C5	121.9 (4)	C17—C18—H18	119.9
C3—C4—H4	119.0	C20—C19—C18	118.8 (7)
C5—C4—H4	119.0	C20—C19—H19	120.6
C4—C5—C6	117.5 (4)	C18—C19—H19	120.6
C4—C5—H5	121.3	C19—C20—C21	122.0 (6)
C6—C5—H5	121.3	C19—C20—H20	119.0
C1—C6—C5	120.1 (4)	C21—C20—H20	119.0

C1—C6—C7	107.2 (3)	C20—C21—C22	120.0 (6)
C5—C6—C7	132.6 (4)	C20—C21—H21	120.0
C8—C7—C6	108.5 (3)	C22—C21—H21	120.0
C8—C7—C23	129.2 (3)	C21—C22—C17	118.4 (6)
C6—C7—C23	121.8 (3)	C21—C22—H22	120.8
C7—C8—N1	107.9 (3)	C17—C22—H22	120.8
C7—C8—C9	126.8 (3)	O5—C23—C7	120.4 (4)
N1—C8—C9	125.2 (3)	O5—C23—C24	121.4 (4)
C10—C9—C8	121.0 (3)	C7—C23—C24	117.9 (3)
C10—C9—H9	119.5	C23—C24—Br1	112.6 (3)
C8—C9—H9	119.5	C23—C24—H24A	109.1
C9—C10—C11	125.5 (3)	Br1—C24—H24A	109.1
C9—C10—H10	117.3	C23—C24—H24B	109.1
C11—C10—H10	117.3	Br1—C24—H24B	109.1
C12—C11—C16	116.1 (3)	H24A—C24—H24B	107.8
C12—C11—C10	119.8 (3)	C8—N1—C1	108.6 (3)
C16—C11—C10	124.0 (3)	C8—N1—S1	125.4 (2)
C13—C12—C11	121.9 (4)	C1—N1—S1	121.7 (2)
C13—C12—H12	119.0	O4—N2—O3	121.1 (4)
C11—C12—H12	119.0	O4—N2—C16	118.5 (4)
C12—C13—C14	120.3 (4)	O3—N2—C16	120.1 (4)
C12—C13—H13	119.8	O2—S1—O1	120.4 (2)
C14—C13—H13	119.8	O2—S1—N1	106.46 (17)
C15—C14—C13	119.6 (4)	O1—S1—N1	105.34 (19)
C15—C14—H14	120.2	O2—S1—C17	109.5 (2)
C13—C14—H14	120.2	O1—S1—C17	109.5 (2)
C14—C15—C16	119.8 (4)	N1—S1—C17	104.24 (17)
C14—C15—H15	120.1		
C6—C1—C2—C3	0.4 (6)	C17—C18—C19—C20	-0.8 (8)
N1—C1—C2—C3	-179.1 (4)	C18—C19—C20—C21	0.1 (9)
C1—C2—C3—C4	0.0 (7)	C19—C20—C21—C22	0.3 (9)
C2—C3—C4—C5	-0.7 (7)	C20—C21—C22—C17	0.0 (8)
C3—C4—C5—C6	1.0 (6)	C18—C17—C22—C21	-0.7 (7)
C2—C1—C6—C5	0.0 (6)	S1—C17—C22—C21	-179.3 (4)
N1—C1—C6—C5	179.6 (3)	C8—C7—C23—O5	-146.1 (4)
C2—C1—C6—C7	-178.3 (4)	C6—C7—C23—O5	42.6 (6)
N1—C1—C6—C7	1.3 (4)	C8—C7—C23—C24	39.2 (6)
C4—C5—C6—C1	-0.7 (5)	C6—C7—C23—C24	-132.1 (4)
C4—C5—C6—C7	177.1 (4)	O5—C23—C24—Br1	-25.8 (6)
C1—C6—C7—C8	-2.4 (4)	C7—C23—C24—Br1	148.9 (3)
C5—C6—C7—C8	179.6 (4)	C7—C8—N1—C1	-1.6 (4)
C1—C6—C7—C23	170.6 (3)	C9—C8—N1—C1	175.4 (3)
C5—C6—C7—C23	-7.4 (6)	C7—C8—N1—S1	-158.3 (3)
C6—C7—C8—N1	2.4 (4)	C9—C8—N1—S1	18.7 (5)
C23—C7—C8—N1	-169.8 (4)	C6—C1—N1—C8	0.2 (4)
C6—C7—C8—C9	-174.6 (3)	C2—C1—N1—C8	179.7 (4)
C23—C7—C8—C9	13.2 (6)	C6—C1—N1—S1	157.9 (2)
C7—C8—C9—C10	41.5 (6)	C2—C1—N1—S1	-22.6 (6)

N1—C8—C9—C10	-135.1 (4)	C15—C16—N2—O4	19.0 (8)
C8—C9—C10—C11	-172.1 (4)	C11—C16—N2—O4	-162.0 (7)
C9—C10—C11—C12	34.8 (6)	C15—C16—N2—O3	-154.8 (5)
C9—C10—C11—C16	-148.3 (4)	C11—C16—N2—O3	24.3 (7)
C16—C11—C12—C13	-0.1 (5)	C8—N1—S1—O2	-32.0 (3)
C10—C11—C12—C13	177.0 (4)	C1—N1—S1—O2	174.2 (3)
C11—C12—C13—C14	0.1 (6)	C8—N1—S1—O1	-160.9 (3)
C12—C13—C14—C15	0.3 (7)	C1—N1—S1—O1	45.2 (3)
C13—C14—C15—C16	-0.7 (7)	C8—N1—S1—C17	83.8 (3)
C14—C15—C16—C11	0.8 (6)	C1—N1—S1—C17	-70.1 (3)
C14—C15—C16—N2	179.8 (4)	C18—C17—S1—O2	22.6 (4)
C12—C11—C16—C15	-0.3 (6)	C22—C17—S1—O2	-158.8 (3)
C10—C11—C16—C15	-177.3 (4)	C18—C17—S1—O1	156.7 (4)
C12—C11—C16—N2	-179.4 (4)	C22—C17—S1—O1	-24.7 (4)
C10—C11—C16—N2	3.7 (6)	C18—C17—S1—N1	-91.0 (4)
C22—C17—C18—C19	1.1 (7)	C22—C17—S1—N1	87.6 (4)
S1—C17—C18—C19	179.6 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 \cdots O5 ⁱ	0.93	2.38	3.147 (5)	139
C2—H2 \cdots O1	0.93	2.38	2.957 (6)	120
C9—H9 \cdots O2	0.93	2.47	2.827 (5)	103
C10—H10 \cdots O3	0.93	2.37	2.730 (5)	103

Symmetry code: (i) $x-1/2, -y+1, z-1/2$.