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

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In the title compound $C_{24}H_{17}BrN_2O_5S$, 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 C—H···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).
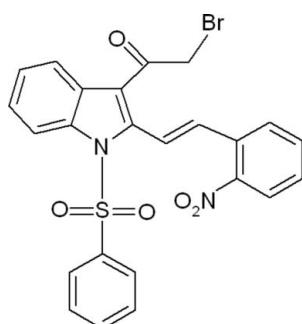
Experimental

Crystal data

$C_{24}H_{17}BrN_2O_5S$	$V = 1110.08$ (15) Å^3
$M_r = 525.37$	$Z = 2$
Monoclinic, Pn	Mo $K\alpha$ radiation
$a = 10.1823$ (7) Å	$\mu = 1.99$ mm^{-1}
$b = 8.0932$ (6) Å	$T = 295$ K
$c = 13.8111$ (12) Å	$0.35 \times 0.25 \times 0.25$ mm
$\beta = 102.749$ (2)°	

Data collection

Bruker APEXII CCD diffractometer	17011 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	4323 independent reflections
$T_{min} = 0.543$, $T_{max} = 0.609$	3368 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	$\Delta\rho_{max} = 0.85$ e Å^{-3}
$wR(F^2) = 0.116$	$\Delta\rho_{min} = -0.43$ e Å^{-3}
$S = 1.01$	Absolute structure: Flack (1983), 2093 Friedel pairs
4323 reflections	Absolute structure parameter: 0.022 (9)
298 parameters	
2 restraints	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5^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*.

References

Andreani, A., Granaiola, M., Leoni, A., Locatelli, A., Morigi, R., Rambaldi, M., Giorgi, G., Salvini, L. & Garaliene, V. (2001). *Anticancer Drug. Des.* **16**, 167–174.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kanchanadevi, J., Anbalagan, G., Saravanan, V., Mohanakrishnan, A. K., Gunasekaran, B. & Manivannan, V. (2014). *Acta Cryst.* E**70**, o148.
Pomarnacka, E. & Kozlarska-Kedra, I. (2003). *Il Farmaco*, **58**, 423–429.
Sheldrick, G. M. (1996). *SADABS*, University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, U. P., Sarma, B. K., Mishra, P. K. & Ray, A. B. (2000). *Fol. Microbiol.* **45**, 173–176.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Srivastava, A. & Pandeya, S. N. (2011). *JCPR*, **1**, 1–17.
Umadevi, M., Saravanan, V., Yamuna, R., Mohanakrishnan, A. K. & Chakkaravarthi, G. (2013). *Acta Cryst.* E**69**, o1784.

supporting information

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

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S1. 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)° and 8.8 (2)° with the indole ring system and the nitro benzene ring, respectively. The sum of bond angles around the atom N1 [355.7°] indicates sp^2 hybridization. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is controlled by weak intermolecular C—H···O interaction.

S2. 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 ° 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)-1*H*- indol-3-yl)ethanone as a yellow solid (0.92 g, 78%) with melting point 184–186 ° C.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.97 Å and U_{iso}(H) = 1.2Ueq(C) for CH$_2$.
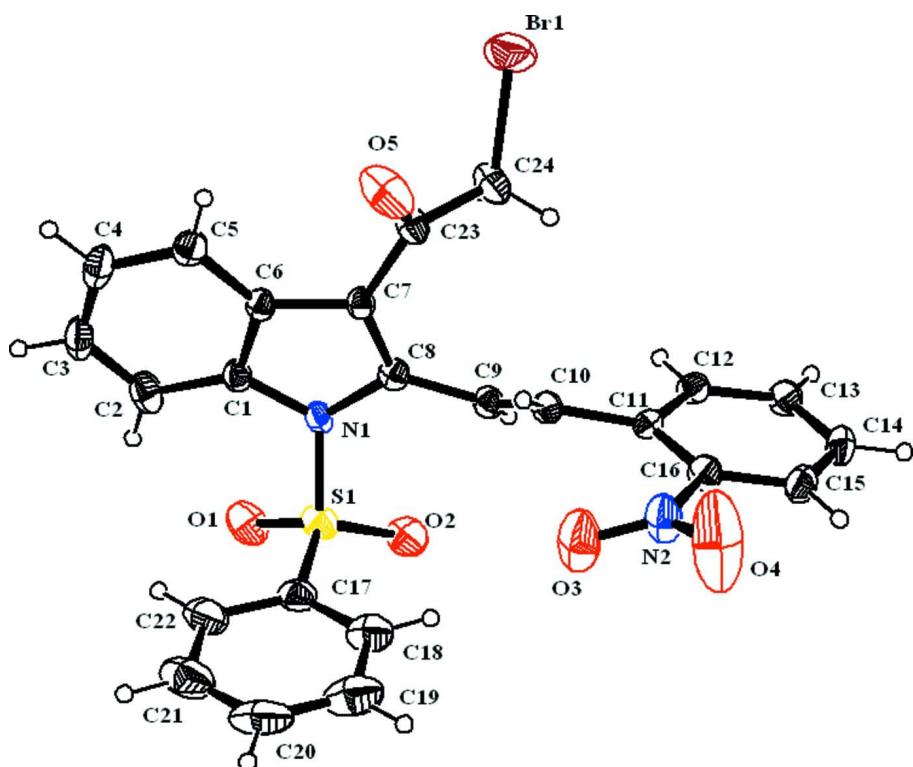
Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.
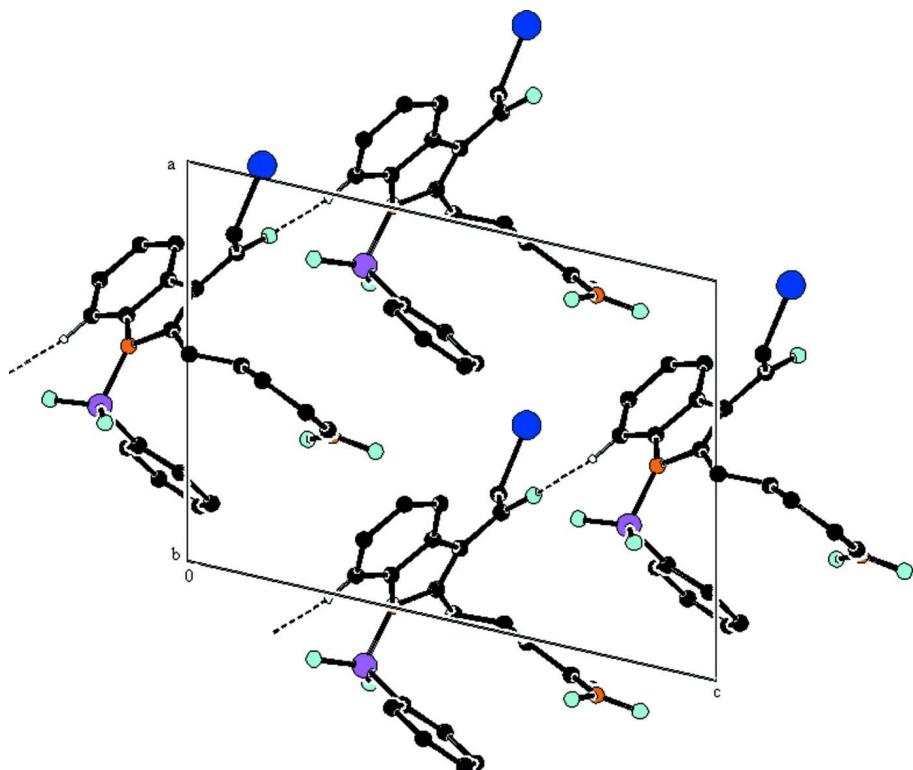
Figure 2
The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{24}H_{17}BrN_2O_5S$	$F(000) = 532$
$M_r = 525.37$	$D_x = 1.572$ Mg m^{-3}
Monoclinic, Pn	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P -2yac	Cell parameters from 4350 reflections
$a = 10.1823$ (7) Å	$\theta = 2.3$–$26.3°$
$b = 8.0932$ (6) Å	$\mu = 1.99$ mm^{-1}
$c = 13.8111$ (12) Å	$T = 295$ K
$\beta = 102.749$ (2)°	Block, yellow
$V = 1110.08$ (15) Å^3	$0.35 \times 0.25 \times 0.25$ mm
$Z = 2$	

Data collection

Bruker APEXII CCD diffractometer	17011 measured reflections
Radiation source: fine-focus sealed tube	4323 independent reflections
Graphite monochromator	3368 reflections with $I > 2\sigma(I)$
Detector resolution: 0 pixels mm^{-1}	$R_{int} = 0.027$
ω and φ scans	$\theta_{max} = 26.3°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -12 \rightarrow 12$
	$k = -9 \rightarrow 9$
$T_{min} = 0.543$, $T_{max} = 0.609$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.3412P]$
$wR(F^2) = 0.116$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4323 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
2 restraints	Absolute structure: Flack (1983), 2093 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.022 (9)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{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 (Å²)

	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, º)

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, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C2—H2⋯O5[i]	0.93	2.38	3.147 (5)	139
C2—H2⋯O1	0.93	2.38	2.957 (6)	120
C9—H9⋯O2	0.93	2.47	2.827 (5)	103
C10—H10⋯O3	0.93	2.37	2.730 (5)	103

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