



# The crystal structures and Hirshfeld surface analysis of three new bromo-substituted 3-methyl-1-(phenylsulfonyl)-1*H*-indole derivatives

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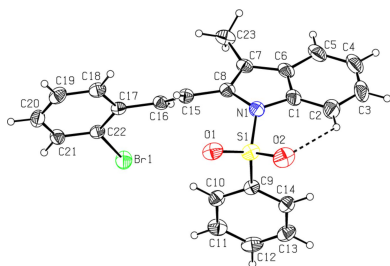
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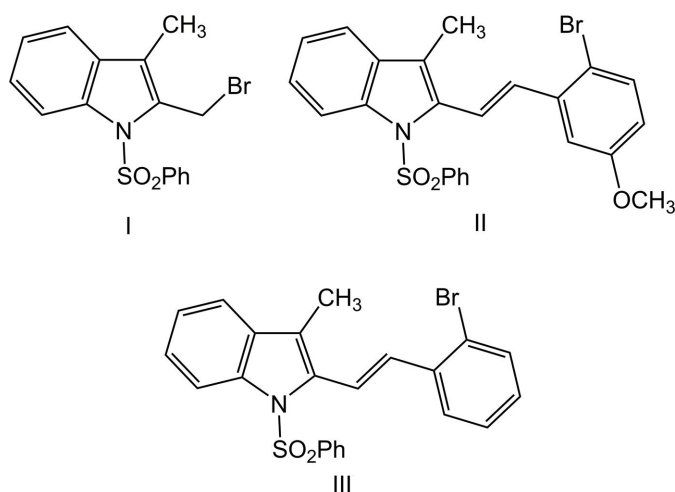
Three new 1*H*-indole derivatives, namely, 2-(bromomethyl)-3-methyl-1-(phenylsulfonyl)-1*H*-indole, C<sub>16</sub>H<sub>14</sub>BrNO<sub>2</sub>S, (**I**), 2-[(*E*)-2-(2-bromo-5-methoxyphenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole, C<sub>24</sub>H<sub>20</sub>BrNO<sub>3</sub>S, (**II**), and 2-[(*E*)-2-(2-bromophenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole, C<sub>23</sub>H<sub>18</sub>BrNO<sub>2</sub>S, (**III**), exhibit nearly orthogonal orientations of their indole ring systems and sulfonyl-bound phenyl rings. Such conformations are favourable for intermolecular bonding involving sets of slipped  $\pi$ - $\pi$  interactions between the indole systems and mutual C—H $\cdots$  $\pi$  hydrogen bonds, with the generation of two-dimensional monophasic patterns. The latter are found in all three structures, in the form of supramolecular columns with every pair of successive molecules related by inversion. The crystal packing of the compounds is additionally stabilized by weaker slipped  $\pi$ - $\pi$  interactions between the outer phenyl rings (in **II** and **III**) and by weak C—H $\cdots$ O, C—H $\cdots$ Br and C—H $\cdots$  $\pi$  hydrogen bonds. The structural significance of the different kinds of interactions agree with the results of a Hirshfeld surface analysis and the calculated interaction energies. In particular, the largest interaction energies (up to  $-60.8$  kJ mol<sup>-1</sup>) are associated with pairing of antiparallel indole systems, while the energetics of weak hydrogen bonds and phenyl  $\pi$ - $\pi$  interactions are comparable and account for 13–34 kJ mol<sup>-1</sup>.

## 1. Chemical context

Derivatives of indole exhibit antibacterial (Okabe & Adachi, 1998) and antitumour (Schollmeyer *et al.*, 1995) activities. In particular, 1-(phenylsulfonyl)indoles are applicable to the synthesis of biologically active alkaloids and their analogues, including pyridocarbazoles, such as the anticancer alkaloid ellipticine, carbazoles, furoindoles, pyrroloindoles, indolo-carbazoles and other species. Some of the phenylsulfonyl indole compounds have been shown to inhibit the HIV-1 RT enzyme *in vitro* and HTLVIIIb viral spread in MT-4 human T-lymphoid cells (Williams *et al.*, 1993). In such systems, the phenylsulfonyl moiety may act either as a protecting or an activating group (Jasinski *et al.*, 2009). Since the related halogen-substituted indoles also demonstrate antibacterial and antifungal activity (Piscopo *et al.*, 1990), one can anticipate a range of functional benefits from the halogen derivatization. Thus, substitution by bromine atoms may significantly enhance *in vitro* blood–brain barrier permeability, providing evidence for improved delivery to the central nervous system (Bouthenet *et al.*, 2011). Bromination on the phenol ring is important for the antimicrobial activity (Gentry *et al.*, 1999). The incorporation of heavy atoms, such as

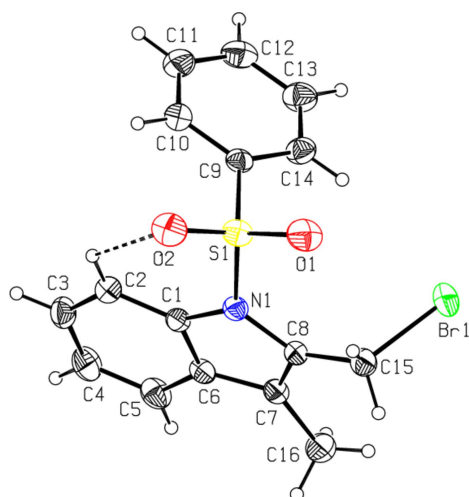


bromine, increases the generation of reactive species during photosensitization (Semenova *et al.*, 2021). In particular, fluorescent Br-substituted dyes are utilized for photodynamic therapy applications (Liu *et al.*, 2021). The fluorescent 4,6-dibromoindolenine cyanine revealed excellent properties for optical tumour imaging (Guerrero *et al.*, 2017). Recognizing the importance of such compounds for biochemical applications and drug discovery and our ongoing research into the construction of indole derivatives have prompted us to investigate a series of Br-substituted species. We report herein the crystal structures determination and Hirshfeld surface analysis of three new indoles: 2-(bromomethyl)-3-methyl-1-(phenylsulfonyl)-1*H*-indole,  $C_{16}H_{14}BrNO_2S$ , (**I**), 2-[(*E*)-2-(2-bromo-5-methoxyphenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole,  $C_{24}H_{20}BrNO_3S$ , (**II**), and 2-[(*E*)-2-(2-bromophenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole (**III**).



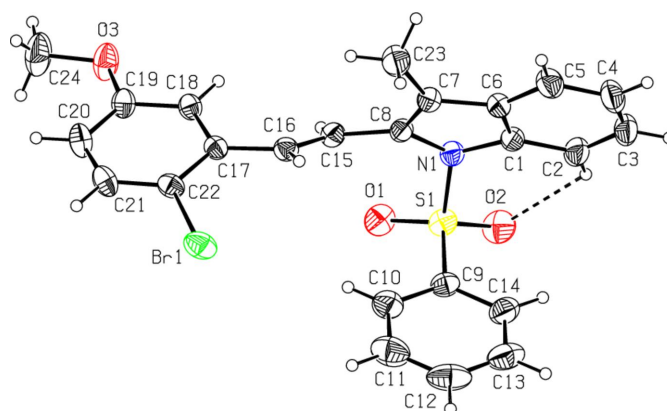
## 2. Structural commentary

The molecular structures of the title compounds,  $C_{16}H_{14}BrNO_2S$ , (**I**),  $C_{24}H_{20}BrNO_3S$ , (**II**) and  $C_{23}H_{18}BrNO_2S$ ,



**Figure 1**

The molecular structure of compound **I**, with atom labelling and displacement ellipsoids drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

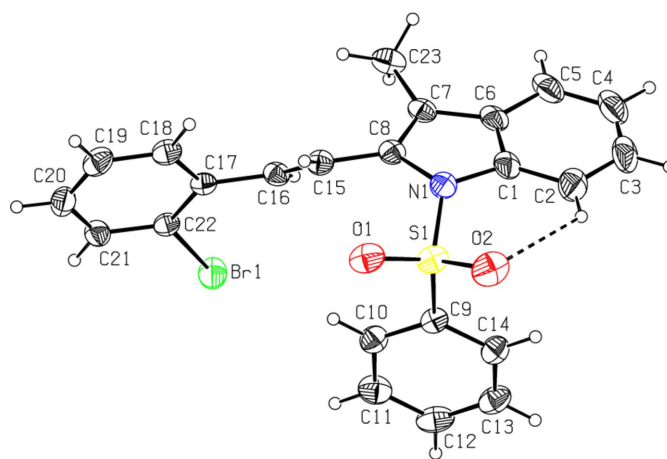


**Figure 2**

The molecular structure of compound **II**, with atom labelling and displacement ellipsoids drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

(**III**), are illustrated in Figs. 1, 2 and 3, respectively. In all the cases, the indole ring systems (N1/C1–C8) are essentially planar, with a maximum deviation from the corresponding mean plane of 0.0393 (17) Å, observed for N1 atom in **III**. The sulfonyl-bound phenyl rings (C9–C14) are almost orthogonal to the carrier indole ring systems (N1/C1–C8), with respective interplanar angles of 76.40 (9)° for **I**, 73.35 (7)° for **II** and 87.68 (8)° for **III**. The ethenyl-bound phenyl rings (C17–C22) in **II** and **III** are also actually orthogonal to the indole frameworks, subtending dihedral angles of 72.48 (7) and 79.50 (8)°, respectively. As a consequence, the planes of these outer phenyl rings (C9–C14 and C17–C22) are nearly parallel, subtending angles of 9.56 (16) in **II** and 18.45 (6)° in **III**.

The torsion angles O2–S1–N1–C1 and O1–S1–N1–C8 [55.3 (2) and –21.1 (2)°, respectively, for **I**, –46.74 (19) and 45.94 (19)° for **II** and 42.9 (2) and –41.8 (2)° for **III**] indicate the *syn* conformation of the sulfonyl moiety. In all three compounds, the tetrahedral configuration around S1 atom is somewhat distorted. The increase in the O2–S1–O1 angles [120.11 (14)° for **I**, 119.67 (12)° for **II** and



**Figure 3**

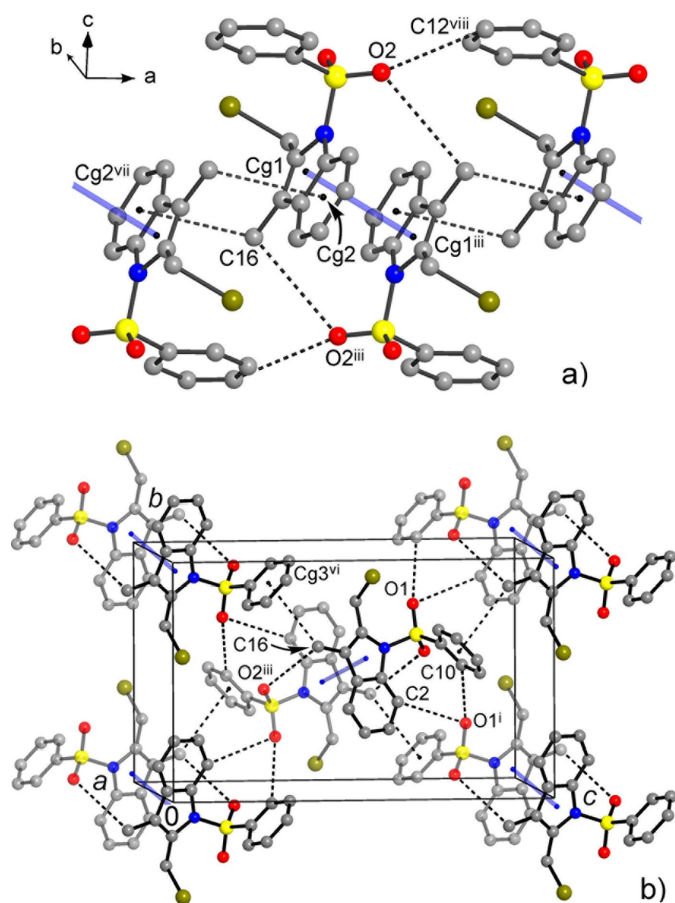
The molecular structure of compound **III**, with atom labelling and displacement ellipsoids drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

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

D—H...A	D—H	H...A	D...A	D—H...A
C2—H2...O2	0.93	2.49	3.057 (4)	120
C2—H2...O1 <sup>i</sup>	0.93	2.71	3.503 (4)	144
C10—H10...O1 <sup>i</sup>	0.93	2.53	3.306 (4)	141
C12—H12...O2 <sup>ii</sup>	0.93	2.77	3.302 (5)	118
C13—H13...O2 <sup>ii</sup>	0.93	2.92	3.376 (4)	112
C16—H16C...O2 <sup>iii</sup>	0.96	2.76	3.702 (4)	168
C4—H4...Br1 <sup>iv</sup>	0.93	3.16	3.905 (4)	138
C12—H12...Br1 <sup>v</sup>	0.93	3.16	3.922 (4)	141
C14—H14...Br1	0.93	2.99	3.894 (4)	165
C16—H16A...Cg(C9—C14) <sup>vi</sup>	0.96	2.97	3.765 (4)	142
C16—H16B...Cg(C1—C6) <sup>vii</sup>	0.96	2.97	3.823 (5)	149

Symmetry codes: (i)  $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $x - 1, y, z$ ; (iii)  $-x + 1, -y + 1, -z + 1$ ; (iv)  $x, y - 1, z$ ; (v)  $-x, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (vi)  $x, y + \frac{3}{2}, z - \frac{1}{2}$ ; (vii)  $-x, -y + 1, -z + 1$ .

119.60 (13)° for **III**], with a simultaneous decrease in the N1—S1—C9 angles [104.46 (12)° for **I**, 103.78 (10)° for **II** and 105.70 (10)° for **III**] from the ideal tetrahedral value (109.5°) are attributed to the Thorpe–Ingold effect (Bassindale, 1984). The widening of the angles may be due to the repulsive interaction between the two short S=O bonds.



**Figure 4**  
(a) Fragment of the structure of **I** showing a column of molecules, down the *a*-axis in the crystal, sustained by  $\pi$ – $\pi$  interactions and weak CH... $\pi$  and CH...O bonds. (b) Projection of the structure nearly down the *a*-axis showing weak CH...O bonds between the columns (which are orthogonal to the drawing plane). Light-blue lines indicate the  $\pi$ – $\pi$  interactions. [Symmetry codes: (i)  $x + 1, y - \frac{1}{2}, -z + 1.5$ ; (iii)  $x + 1, -y + 1, -z + 1$ ; (vi)  $x, -y + 1.5, z - \frac{1}{2}$ ; (vii)  $-x, -y + 1, -z + 1$ ; (viii)  $x + 1, y, z$ .]

**Table 2**  
Hydrogen-bond geometry (Å, °) for **II**.

D—H...A	D—H	H...A	D...A	D—H...A
C2—H2...O2	0.93	2.39	2.958 (4)	119
C3—H3...O2 <sup>i</sup>	0.93	2.61	3.448 (3)	150
C24—H24A...Br1 <sup>ii</sup>	0.96	3.03	3.699 (3)	128
C5—H5...Cg(C9—C14) <sup>iii</sup>	0.93	3.12	4.047 (3)	173
C20—H20...Cg(C17—C22) <sup>iv</sup>	0.93	3.15	3.978 (2)	149
C23—H23C...Cg(C1—C6) <sup>iii</sup>	0.96	3.11	4.036 (4)	162

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

**Table 3**  
Hydrogen-bond geometry (Å, °) for **III**.

D—H...A	D—H	H...A	D...A	D—H...A
C2—H2...O2	0.93	2.37	2.949 (5)	120
C13—H13...O1 <sup>i</sup>	0.93	2.73	3.420 (3)	132
C14—H14...O2 <sup>ii</sup>	0.93	2.77	3.547 (4)	142
C19—H19...Br1 <sup>iii</sup>	0.93	2.94	3.805 (3)	155
C5—H5...Cg(C9—C14) <sup>iv</sup>	0.93	2.96	3.806 (4)	153
C23—H23A...Cg(C1—C6) <sup>iv</sup>	0.96	3.21	3.999 (3)	110
C23—H23B...Cg(N1/C1/C6—C8) <sup>v</sup>	0.96	3.12	3.561 (3)	149

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

In all three compounds, the sum of the bond angles around N1 [355.88 (11), 348.62 (17) and 352.89 (12)° for **I**, **II** and **III**, respectively] indicate  $sp^2$  hybridization (Beddoes *et al.*, 1986). At the same time, as a result of the electron-withdrawing character of the phenylsulfonyl groups, the N1—C $sp^2$  bonds are longer than the standard length value of 1.355 (14) Å [N1—C1 = 1.419 (3) for **I**, 1.425 (3) for **II** and 1.428 (3) Å for **III** and N1—C8 = 1.434 (3) for **I**, 1.438 (3) for **II** and 1.437 (3) Å for **III**] (Allen *et al.*, 1987; Cambridge Structural Database (CSD), Version 5.37; Groom *et al.*, 2016). In all the compounds, the certain expansion of the *ipso* angles at atoms C1, C3 and C4, and the contraction of the apical angles at atoms C2, C5 and C6 are caused by fusion of the smaller pyrrole ring with the six-membered benzene ring and the strain is taken up by the angular distortion rather than by bond-length distortion (Allen, 1981). The geometric parameters of the present compounds agree well with those reported for related structures (Madhan *et al.*, 2022, 2023a,b). In all three compounds, the molecular conformations are stabilized by weak C2—H2...O2 intramolecular interactions with C2...O2 = 2.950 (2)–3.057 (4) Å.

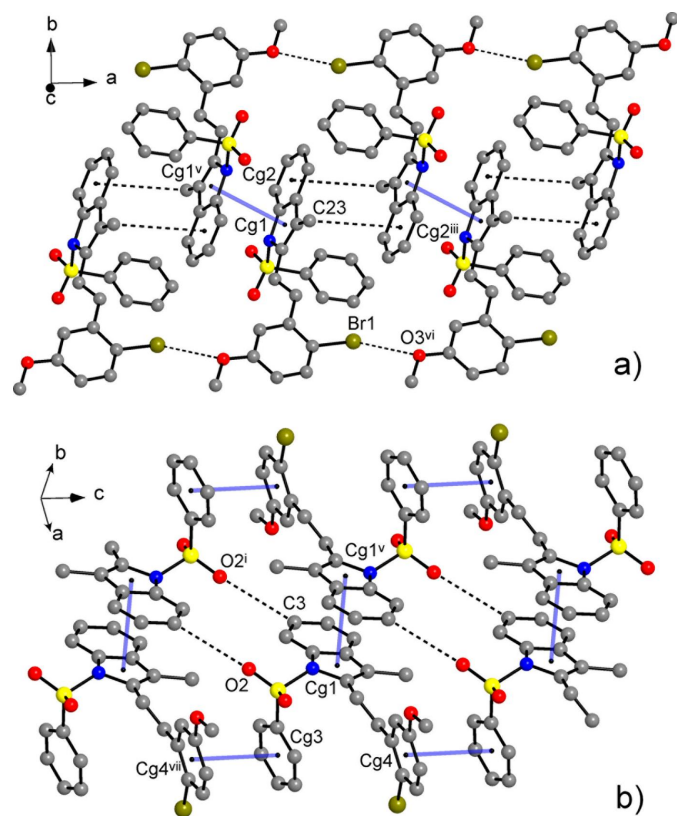
### 3. Supramolecular features

With a lack of conventional hydrogen-bond donor functionality, the supramolecular structures of all three compounds are dominated by weaker interactions, namely by weak C—H...O, C—H...Br and C—H... $\pi$  hydrogen bonds (Tables 1–3) and slipped  $\pi$ – $\pi$  stacking interactions (Table 4).

In the structure of **I**, molecules are linked *via* double bonds involving C2—H2 and C10—H10 donors and O1<sup>i</sup> acceptors [C...O = 3.306 (4) and 3.503 (4) Å; symmetry code: (i)  $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ ] into the chains propagating along the *b*-axis direction in the crystal (Table 1). The most salient feature of the array is infinite stacking of the indole moieties, which yields columns down the *a*-axis. Within these columns, pairs of

adjacent molecules are held together by  $\pi$ - $\pi$  interactions or by double  $\text{CH}_3 \cdots \pi$  bonds, in alternate sequence (Fig. 4). The counterparts of every such pairs are related by inversion [symmetry codes: (iii)  $-x + 1, -y + 1, -z + 1$ ; (v)  $-x, -y + 1, -z + 1$ , respectively.] For the dimer of the first kind, the geometry parameters are consistent with weak slipped  $\pi$ - $\pi$  interactions. The shortest intercentroid distance is observed between the pyrrole rings (Table 4). However, the centroid of the N1/C1-C8 group (Cg1) is situated almost above the midpoint of the C1 and C6 bridgehead atoms of the neighbouring molecule and therefore both pyrrole-pyrrole [ $\text{Cg1} \cdots \text{Cg1}^{\text{iii}} = 3.628$  (3) Å] and pyrrole-benzo [ $\text{Cg1} \cdots \text{Cg2}^{\text{iii}} = 3.831$  (3) Å] interactions may be considered. The entire  $\pi$ - $\pi$  and  $\text{CH}_3 \cdots \pi$  bonded stack is additionally stabilized by weak hydrogen bonding of the sulfonyl O atoms [ $\text{C} \cdots \text{O} = 3.302$  (5)– $3.702$  (4) Å]. One can note the functional importance of the methyl group, which is a donor of three highly directional interactions, *viz.* the  $\text{C}-\text{H} \cdots \text{O}$  bond and two  $\text{C}-\text{H} \cdots \pi$  bonds (Table 1).

The structure of **II** inherits the above motif (Fig. 5). In particular, a combination of  $\pi$ - $\pi$  and  $\text{CH}_3 \cdots \pi$  interactions assembles the molecules into columns propagating along the *a*-axis direction in the crystal, in exactly the same manner as observed for compound **I**. In this case, the interactions are

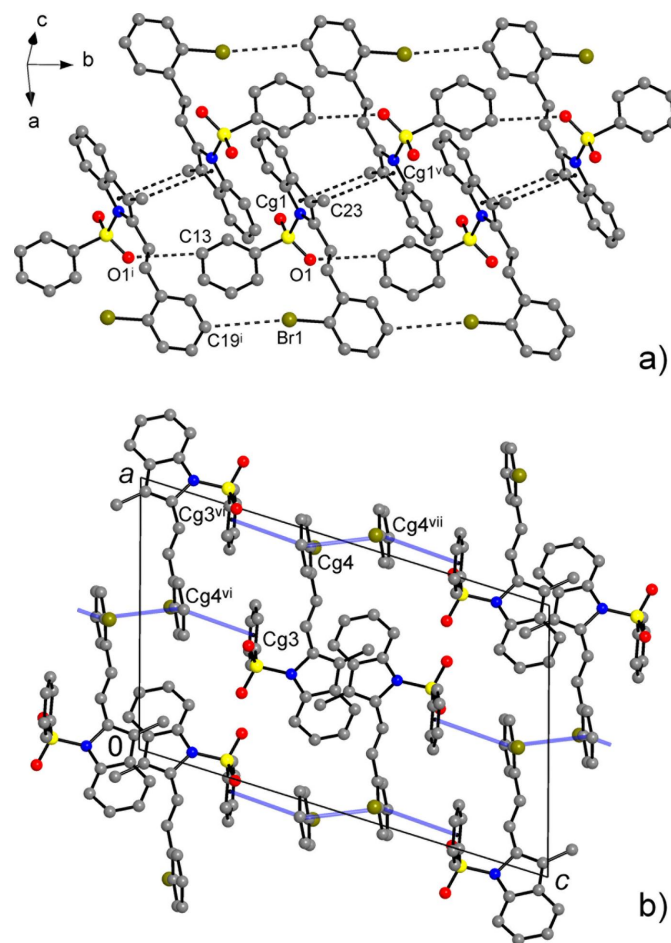


**Figure 5**

(a) Fragment of the structure of **II**, with columns of the molecules down the *a*-axis, held by  $\pi$ - $\pi$  (represented by light blue lines) and  $\text{CH} \cdots \pi$  bonds. Short  $\text{Br1} \cdots \text{O3}^{\text{vi}}$  contacts [3.3066 (19) Å] are also shown. (b) Projection of the structure on the *ac*-plane. Note the extensive  $\pi$ - $\pi$  interactions of the phenyl rings yielding four-decker sandwiches. The indole columns are orthogonal to the drawing plane. [Symmetry codes: (i)  $x + 1, -y + 1, -z$ ; (iii)  $x + 2, -y + 1, -z + 1$ ; (v)  $x + 1, -y + 1, -z + 1$ ; (vi)  $x + 1, y, z$ ; (vii)  $x, y, z - 1$ .]

slightly weaker and the corresponding intercentroid distances [ $\text{Cg1} \cdots \text{Cg1}^{\text{v}} = 3.692$  (3) Å; symmetry code: (v)  $-x + 1, -y + 1, -z + 1$ ] are slightly larger compared with **II** (Table 4). The outer 2-bromo-5-methoxyphenyl rings also contribute to the packing pattern since they afford  $\pi$ - $\pi$  interactions with the sulfonyl-bound C9-C14 rings, with typical intercentroid separations of 3.836 (2) Å and a relatively small slippage angle of 18.1 (2)° (Table 4). This stacking complements the weak  $\text{C3}-\text{H3} \cdots \text{O2}^{\text{i}}$  hydrogen bonds [ $\text{C} \cdots \text{O} = 3.448$  (3) Å; symmetry code: (i)  $-x + 1, -y + 1, -z$ ], linking the columns of molecules in the *c*-axis direction (Fig. 5). There are no hydrogen-bonding interactions with the methoxy O3 atoms, which instead are involved in relatively short  $\text{Br} \cdots \text{O}$  contacts of 3.3066 (19) Å. Very distal contacts of the type  $\text{C24} \cdots \text{Cg4}^{\text{ix}}$  [4.098 (3) Å; Cg4 is the ring C17-C22 centroid; symmetry code: (ix)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ] possibly indicate weak  $\text{C}-\text{H} \cdots \pi$  interactions.

In the structure of **III**, the  $\pi$ - $\pi$  interactions of the indole ring systems are eliminated since the shortest intercentroid



**Figure 6**

(a) Fragment of the structure of **III**, showing mutual  $\text{CH} \cdots \pi$  bonding of the inversion-related indole fragments and how  $\text{CH} \cdots \text{O}$  and  $\text{CH} \cdots \text{Br}$  bonds contribute to the stabilization of the supramolecular column. (b) Projection of the structure on the *ac*-plane. Note the extensive  $\pi$ - $\pi$  interactions of the phenyl rings yielding four-decker sandwiches. The indole columns are orthogonal to the drawing plane. [Symmetry codes: (i)  $x, y - 1, z$ ; (v)  $x + 1, -y + 2, -z + 1$ ; (vi)  $x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (vii)  $x + 2, -y + 2, -z + 1$ .]

**Table 4**  
Geometry of stacking interactions (Å, °) for **I–III**.

$Cg$  is a group centroid;  $\text{plane} \cdots CgB$  is the distance between the mean plane of Group  $A$  and the centroid of the interacting Group  $B$ ; ipa is the interplanar angle; sa is the slippage angle, which is the angle of the  $CgA \cdots CgB$  axis to the Group  $A$  mean plane normal.

Compound	Group $A$	Group $B$	Shortest contacts	$CgA \cdots CgB$	Plane $\cdots CgB$	ipa	sa
<b>I</b>	(N1/C1–C8)	(N1/C1–C8) <sup>iii</sup>	3.573 (4)	3.628 (2)	3.551 (2)	0	11.8 (2)
	(N1/C1–C8)	(C1–C6) <sup>iii</sup>	3.573 (4)	3.831 (2)	3.552 (2)	0.16 (14)	22.0 (2)
<b>II</b>	(N1/C1–C8)	(N1/C1–C8) <sup>v</sup>	3.618 (3)	3.692 (2)	3.633 (2)	0	10.3 (2)
	(N1/C1–C8)	(C1–C6) <sup>v</sup>	3.618 (3)	3.975 (2)	3.635 (2)	0.62 (13)	23.9 (2)
	(C17–C22)	(C19–C14) <sup>vii</sup>	3.463 (3)	3.836 (3)	3.646 (3)	9.56 (16)	18.1 (2)
	(C17–C22)	(C9–C14) <sup>vi</sup>	3.381 (3)	3.742 (2)	3.379 (2)	10.34 (7)	24.5 (2)
<b>III</b>	(C17–C22)	(C17–C22) <sup>vii</sup>	3.489 (3)	3.691 (2)	3.488 (2)	0	19.1 (2)

Symmetry codes for **I** (iii)  $-x + 1, -y + 1, -z + 1$ ; for **II**: (v)  $-x + 1, -y + 1, -z + 1$ ; (vii)  $x, y, z - 1$ ; for **III**: (vi)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (vii)  $-x + 2, -y + 2, -z + 1$ .

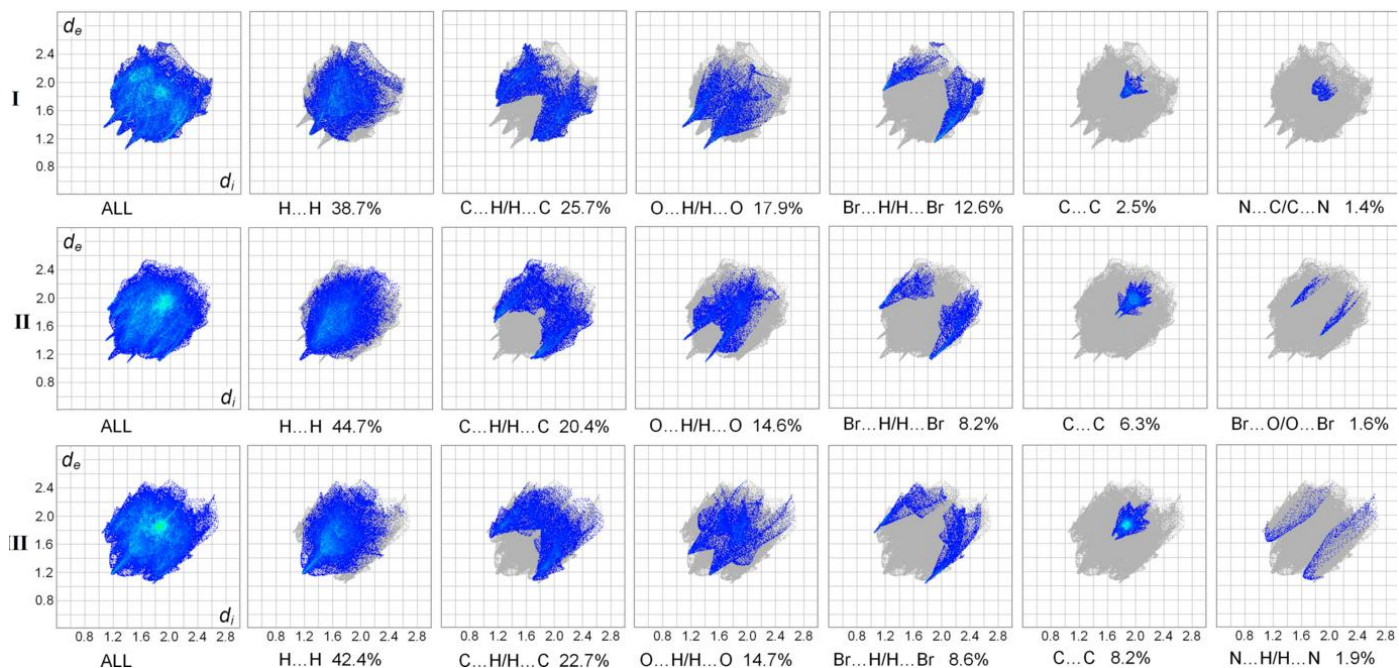
distance exceeds 4.4 Å. However, the structure retains the double  $\text{CH}_3 \cdots \pi$  bonding between inversion-related molecules with  $\text{C23} \cdots Cg1^v = 3.560$  (3) Å [ $Cg1$  is the centroid of the pyrrole ring N1/C1/C6–8; symmetry code: (v)  $-x + 1, -y + 2, -z + 1$ ]. Moreover, these methyl groups also establish distal mutual contacts with the C1–C6 rings [ $\text{C23} \cdots Cg2^{iv} = 3.999$  (3) Å; symmetry code: (iv)  $-x + 1, -y + 1, -z + 1$ ], which likely represent very weak  $\text{CH}_3 \cdots \pi$  bonding. These interactions act in synergy with a set of weak  $\text{C13} \cdots \text{O1}^i$  and  $\text{C19} \cdots \text{H19} \cdots \text{Br1}^{iii}$  bonds (Table 3) to link the molecules into the columns down the  $b$ -axis direction (Fig. 6). Therefore, the main features of the patterns seen for **I** and **II** are preserved for **III** with only minor variations. At the same time, beyond the supramolecular columns, which are nearly intact for all three compounds, the bonding features for **III** are essentially different. Both kinds of the phenyl rings afford a set of  $\pi$ - $\pi$  interactions with the generation of discrete tetramers (Fig. 6), with the central duo representing a stack of two antiparallel inversion-related bromophenyl groups

[ $\text{Cg4} \cdots \text{Cg4}^{vii} = 3.691$  (2) Å; symmetry code: (vii)  $-x + 2, -y + 2, -z + 1$ ]. This central fragment is extended by incorporation of two outer sulfonyl-bound phenyl groups [ $\text{Cg4} \cdots \text{Cg3}^{vi} = 3.742$  (2) Å; symmetry code: (vi)  $-x + \frac{3}{2}, y + 0.5, -z + \frac{1}{2}$ ].

#### 4. Hirshfeld surface analysis

The supramolecular interactions in the title structure were further assessed by Hirshfeld surface analysis. The Hirshfeld surfaces and 2D fingerprint plots were generated using *CystalExplorer21* software (Spackman *et al.*, 2021).

The two-dimensional fingerprint plots (Parkin *et al.*, 2007) detailing the various interactions for the molecules are shown in Fig. 7. For all three compounds, Hirshfeld surfaces suggest the dominance of contacts with the hydrogen atoms, accounting for over 90% of the contacts. Beyond the largest fractions of  $\text{H} \cdots \text{H}$  contacts (38.7–44.7%), the principal



**Figure 7**  
Two-dimensional fingerprint plots for **I–III** and delineated into the principal contributions of  $\text{H} \cdots \text{H}$ ,  $\text{C} \cdots \text{H}/\text{H} \cdots \text{C}$ ,  $\text{O} \cdots \text{H}/\text{H} \cdots \text{O}$ ,  $\text{Br} \cdots \text{H}/\text{H} \cdots \text{Br}$ ,  $\text{C} \cdots \text{C}$ ,  $\text{N} \cdots \text{C}/\text{C} \cdots \text{N}$ ,  $\text{Br} \cdots \text{O}/\text{O} \cdots \text{Br}$  and  $\text{N} \cdots \text{H}/\text{H} \cdots \text{N}$  contacts. Other contributors account for less than 1.0% contacts to the surface areas.

Table 5

Calculated interaction energies (kJ mol<sup>-1</sup>) for **I–III**.

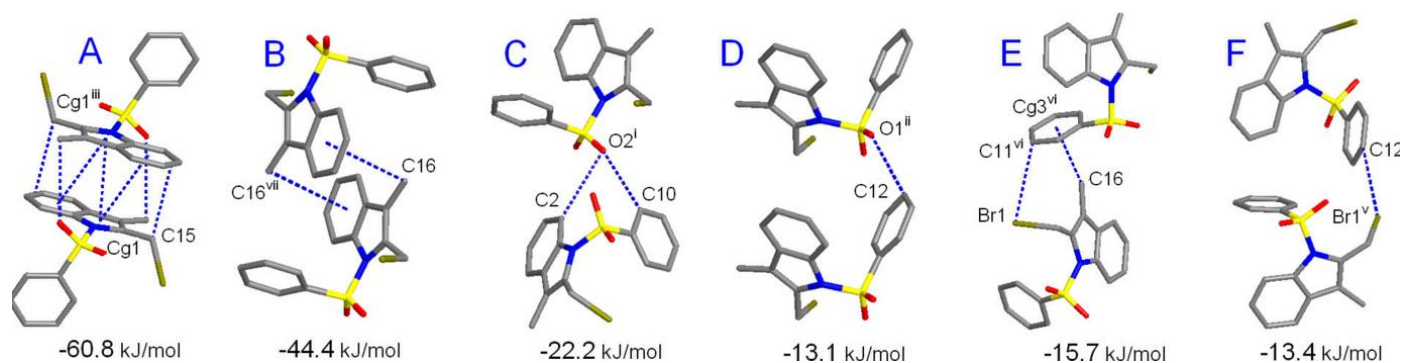
Interaction energies were calculated employing the CE-B3LYP/6-31G(d,p) functional/basis set combination. The scale factors used to determine  $E_{\text{tot}}$  were:  $k_{\text{ele}} = 1.057$ ,  $k_{\text{pol}} = 0.740$ ,  $k_{\text{dis}} = 0.871$ , and  $k_{\text{rep}} = 0.618$  (Mackenzie *et al.*, 2017). For details of the interaction modes, see Figs. 8–10;  $R$  is the distance in Å between the centroids of interacting molecules.

Type	Symmetry code	Interaction	$R$	$E_{\text{ele}}$	$E_{\text{pol}}$	$E_{\text{dis}}$	$E_{\text{rep}}$	$E_{\text{tot}}$
<b>Compound I</b>								
A	$-x + 1, -y + 1, -z + 1$	$\pi$ - $\pi$ , CH $\cdots$ O	6.45	-20.2	-4.5	-71.5	42.4	-60.8
B	$-x, -y + 1, -z + 1$	CH- $\pi$	6.35	-10.5	-2.0	-59.9	32.8	-44.4
C	$-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$	CH $\cdots$ O	7.79	-7.9	-3.6	-22.8	14.0	-22.2
D	$x - 1, y, z$	CH $\cdots$ O	7.98	-5.7	-2.0	-10.6	6.0	-13.1
E	$x, -y + \frac{3}{2}, z - \frac{1}{2}$	CH $\cdots$ Br, CH $\cdots$ $\pi$	9.09	-5.0	-0.9	-18.6	10.4	-15.7
F	$-x, y - \frac{1}{2}, -z + \frac{3}{2}$	CH $\cdots$ Br	9.03	-2.3	-1.0	-17.8	8.5	-13.4
<b>Compound II</b>								
A	$-x + 1, -y + 1, -z + 1$	$\pi$ - $\pi$	8.08	-8.9	-2.9	-67.3	29.0	-52.3
B	$-x + 2, -y + 1, -z + 1$	CH- $\pi$	8.10	-15.7	-1.7	-67.9	44.6	-49.4
C	$-x + 1, -y + 1, -z$	CH $\cdots$ O	12.70	-12.6	-2.9	-15.4	0.0	-28.9
D	$x + 1, y, z$	CH $\cdots$ O	8.43	-7.1	-2.2	-18.7	13.6	-17.1
E	$x, y, z - 1$	$\pi$ - $\pi$	8.95	-4.2	-2.6	-47.8	22.8	-33.9
F	$x, -y + \frac{1}{2}, z - \frac{1}{2}$	CH $\cdots$ Br, CH $\cdots$ $\pi$	8.77	-6.2	-2.2	-38.6	20.2	-29.3
<b>Compound III</b>								
A	$-x + 1, -y + 1, -z + 1$	CH $\cdots$ O, dispersion	7.64	-11.5	-1.9	-78.4	43.3	-55.1
B	$-x + 1, -y + 2, -z + 1$	CH $\cdots$ $\pi$	7.91	-9.3	-2.0	-57.5	29.5	-43.1
C	$-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$	$\pi$ - $\pi$	7.85	-7.1	-1.7	-40.7	21.3	-31.0
D	$-x + 2, -y + 2, -z + 1$	$\pi$ - $\pi$	9.91	-5.2	-1.1	-50.4	34.5	-28.9
E	$x, y - 1, z$	CH $\cdots$ O, CH $\cdots$ Br	8.35	-10.5	-2.7	-28.3	21.7	-24.3
F	$-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$	CH $\cdots$ O	10.52	-3.6	-2.7	-15.6	6.0	-15.7

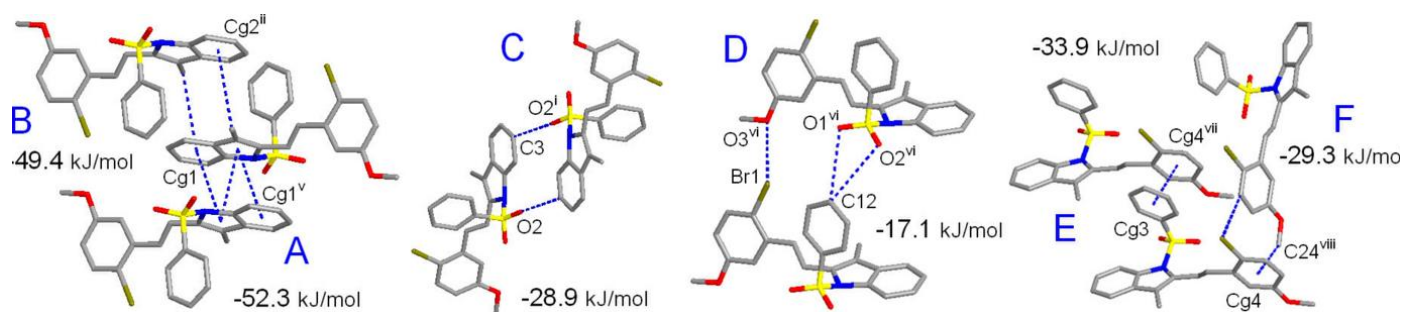
contributors are C $\cdots$ H/H $\cdots$ C (20.4–25.7%), O $\cdots$ H/H $\cdots$ O (14.6–17.9%) and Br $\cdots$ H/H $\cdots$ Br (8.2–12.6%) contacts corresponding to the different kinds of C–H $\cdots$  $\pi$ , C–H $\cdots$ O or C–H $\cdots$ Br bonds. Every type of such bonding is readily identified by the plots representing pairs of diffuse spikes pointing to the lower left. One can note a common trend for suppression of such hydrogen bonding in **II** and **III**. For example, the contribution of the O $\cdots$ H/H $\cdots$ O contacts for **I** (17.9%) is perceptibly larger than for **II** (14.6%), which incorporates an additional methoxy O atom. This effect may be attributed to the increasing significance of  $\pi$ - $\pi$  interactions for the crystal packing in the case of **II** and **III**, in line with the increased number of aromatic groups. In addition, a slight reduction in the Br $\cdots$ H/H $\cdots$ Br contacts (12.6% for **I** versus 8.2% and 8.6% for **II** and **III**, respectively) may be reflective of a weaker acceptor ability of the phenyl-bound Br atoms with respect to the bromomethyl moieties in **I**. An overlap between nearly parallel aromatic frames, due to the slipped  $\pi$ - $\pi$  stacking, is clearly indicated by the C $\cdots$ C plots for all compounds, in the form of the blue–green area centred at  $ca d_e = d_i = 1.85$  Å. The plots suggest a progressive growth of the significance of these interactions, when moving from **I** to **II** and **III**. In line with this, the contributions of the C $\cdots$ C contacts to the entire surfaces are 2.5%, 6.3% and 8.2%, respectively. In the case of **II**, the peculiar short Br $\cdots$ O contacts are also readily identified by the fingerprint plots and they contribute as much as 1.6% to the surface area (Fig. 7).

The interaction energy between the molecules is expressed in terms of four components: electrostatic, polarization, dispersion and exchange repulsion. These energies were obtained using monomer wavefunctions calculated at the B3LYP/6-31G(d,p) level. The total interaction energy, which is the sum of scaled components, was calculated for a 3.8 Å radius cluster of molecules around the selected molecule. The

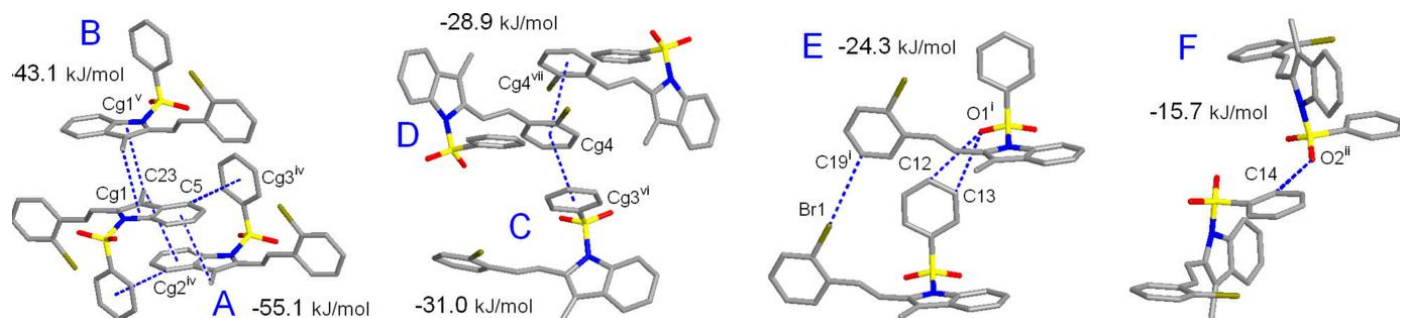
scale factors used in the CE-B3LYP bench research marked energy model (Mackenzie *et al.*, 2017) are given in Table 5. The principal interaction pathways for **I–III** are shown in Figs. 8–10, respectively. The interaction energies calculated by the energy model reveal that the interactions in the crystal have a significant contribution from dispersion components. It is worth noting that the primary forces for the crystal packing are associated with different stackings of the indole moieties. Either  $\pi$ - $\pi$  or double CH $\cdots$  $\pi$  interactions of the inversion-related molecules are equally important and they are particularly prevalent in the case of **I**. Thus, the highest energy  $E_{\text{tot}} = -60.8$  kJ mol<sup>-1</sup> corresponds to the pairing pattern of type A (Fig. 8), with contributions from slipped  $\pi$ - $\pi$  interactions and double C–H $\cdots$ O hydrogen bonding. In addition, short contacts of the methylene groups C15 and C3–C4 bonds [C15 $\cdots$ Cg(C3/C4)<sup>iii</sup> = 3.412 (2) Å; symmetry code: (iii)  $-x + 1, -y + 1, -z + 1$ ] possibly reflect a kind of weak tetrel C $\cdots$  $\pi$  bonding. The energies of other types of indole/indole interactions for **II** and **III** are comparable [ $E_{\text{tot}} = -43.1$  to  $-55.1$  kJ mol<sup>-1</sup>] and the primary contributor here is London dispersion [up to  $-78.4$  kJ mol<sup>-1</sup>], in accordance with the very large interaction areas. The energies of the slipped  $\pi$ - $\pi$  interactions of the phenyl rings in **II** and **III** are very similar and they account for  $-28.9$  to  $-33.9$  kJ mol<sup>-1</sup> (Table 4). The significance of these interactions is comparable with weak C–H $\cdots$ O hydrogen bonds. The energies of the latter themselves are only medium, for example  $-13.1$  kJ mol<sup>-1</sup> (Type D) in **I** and  $-15.7$  kJ mol<sup>-1</sup> (Type F) in **II**. However, pairing of the molecules *via* multiple hydrogen bonding increases the interaction energies up to  $-28.9$  kJ mol<sup>-1</sup> (Type C in **II**, Fig. 9). This rich landscape of bonding modes, with a specific hierarchy of interaction energies, could be applicable as a model for supramolecular interactions of phenylsulfonyl-substituted indoles and their targeting of biomedical substrates.



**Figure 8**  
The principal pathways of the intermolecular interactions for **I** representing  $\pi$ - $\pi$  and weak hydrogen bonding, with a cut-off limit for calculated energies of 6.0 kJ mol<sup>-1</sup>. [Symmetry codes: (i)  $x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $x - 1, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (iii)  $x + 1, -y + 1, -z + 1$ ; (v)  $x, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (vi)  $x, -y + \frac{3}{2}, z - \frac{1}{2}$ .]



**Figure 9**  
The principal pathways of the intermolecular interactions for **II** representing  $\pi$ - $\pi$  and weak hydrogen bonding, with a cut-off limit for calculated energies of 12.0 kJ mol<sup>-1</sup>. [Symmetry codes: (i)  $x + 1, -y + 1, -z$ ; (iii)  $x + 2, -y + 1, -z + 1$ ; (v)  $x + 1, -y + 1, -z + 1$ ; (vi)  $x + 1, y, z$ ; (vii)  $x, y, z - 1$ ; (viii)  $x, -y + \frac{1}{2}, z - \frac{1}{2}$ .]



**Figure 10**  
The principal pathways of the intermolecular interactions for **II** representing  $\pi$ - $\pi$  and weak hydrogen bonding, with a cut-off limit for calculated energies of 6.0 kJ mol<sup>-1</sup>. [Symmetry codes: (i)  $x, y - 1, z$ ; (ii)  $x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (iv)  $x + 1, -y + 1, -z + 1$ ; (v)  $x + 1, -y + 2, -z + 1$ ; (vi)  $x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (vii)  $x + 2, -y + 2, -z + 1$ .]

## 5. Database survey

A search of the Cambridge Structural Database (Version 5.37; Groom *et al.*, 2016), indicated 123 compounds incorporating a phenylsulfonyl-1*H*-indole moiety. Of these compounds, several similar structures have been reported earlier, *i.e.* ethyl 2-acetoxymethyl-1-phenylsulfonyl-1*H*-indole-3-carboxylate (Gunasekaran *et al.*, 2009), 3-iodo-2-methyl-1-phenylsulfonyl-1*H*-indole (Ramathilagam *et al.*, 2011) and 1-(2-bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one (Umadevi *et al.*, 2013). In these structures, the sulfonyl-bound phenyl rings are

almost orthogonal to the indole ring systems, with corresponding dihedral angles of 83.35 (5), 82.84 (9) and 89.91 (11)°, respectively, being comparable with those in the present three compounds.

## 6. Synthesis and crystallization

**Compound I:** To a mixture of *N*-phenylsulfonyl-3-methylindole (6.00 g, 22.22 mmol) and paraformaldehyde (3.33 g, 111.1 mmol) in 50 ml of dry CCl<sub>4</sub>, a 33 wt % solution HBr in

**Table 6**  
Experimental details.

	I	II	III
Crystal data			
Chemical formula	C <sub>16</sub> H <sub>14</sub> BrNO <sub>2</sub> S	C <sub>24</sub> H <sub>20</sub> BrNO <sub>3</sub> S	C <sub>23</sub> H <sub>18</sub> BrNO <sub>2</sub> S
<i>M<sub>r</sub></i>	364.25	482.38	452.35
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>n</i>
Temperature (K)	298	298	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.979 (6), 11.100 (8), 17.540 (14)	8.4252 (9), 28.669 (3), 8.9462 (11)	12.5530 (8), 8.3533 (5), 19.7698 (11)
$\beta$ (°)	99.04 (3)	95.445 (4)	107.078 (2)
<i>V</i> (Å <sup>3</sup> )	1534 (2)	2151.1 (4)	1981.6 (2)
<i>Z</i>	4	4	4
Radiation type	Mo <i>K</i> $\alpha$	Mo <i>K</i> $\alpha$	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	2.82	2.03	2.20
Crystal size (mm)	0.30 × 0.24 × 0.07	0.25 × 0.20 × 0.13	0.36 × 0.31 × 0.24
Data collection			
Diffractometer	Bruker D8 Venture Diffractometer	Bruker D8 Venture Diffractometer	Bruker D8 Venture Diffractometer
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.589, 0.753	0.555, 0.745	0.514, 0.745
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	66991, 4464, 3158	52479, 5296, 3905	50531, 4293, 3516
<i>R</i> <sub>int</sub>	0.049	0.077	0.058
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.704	0.666	0.639
Refinement			
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.046, 0.118, 1.10	0.039, 0.099, 1.03	0.036, 0.087, 1.10
No. of reflections	4464	5296	4293
No. of parameters	191	272	254
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.75, -0.80	0.39, -0.68	0.37, -0.32

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXS2018/3* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2020).

acetic acid (13.46 ml) was added rapidly. The mixture was kept at room temperature for 6 h. After completion of the reaction (monitored by TLC), the mixture was poured into 100 ml of ice–water and then extracted with CCl<sub>4</sub> (2 × 20 ml). The extract was dried with Na<sub>2</sub>SO<sub>4</sub>. Removal of the solvent *in vacuo* followed by crystallization from methanol (4 ml) afforded compound **I** as a colourless solid (yield: 6.9 g, 86%).

**Compound II:** To a suspension of hexane (5 mL) washed NaH (0.43 g, 10.92 mmol) in dry THF (5 ml), a solution of diethyl {[3-methyl-1-(phenylsulfonyl)-1*H*-indol-2-yl]methyl} phosphonate (2.30 g, 5.46 mmol) in dry THF (10 ml) was slowly added *via* an addition funnel at 283 K under an N<sub>2</sub> atmosphere and stirred for 15 min. Then a solution of 2-bromo-5-methoxybenzaldehyde (1.39 g, 6.55 mmol) in dry THF (5 ml) was added and the mixture was allowed to stir for an additional 1 h. After completion of the reaction (monitored by TLC), the mixture was poured over crushed ice (100 g) containing concentrated HCl (1 ml). The solid formed was filtered and washed with methanol. Recrystallization from methanol (4 ml) afforded compound **II** as a bright-yellow solid (yield: 2.00 g, 76%). M.p. = 425–427 K.

**Compound III:** To a suspension of hexane (5 mL) washed NaH (0.38 g, 9.50 mmol) in dry THF (5 ml), a solution of diethyl {[3-methyl-1-(phenylsulfonyl)-1*H*-indol-2-yl]methyl} phosphonate (2.00 g, 4.75 mmol) in dry THF (10 ml) was slowly added *via* an addition funnel at 283 K under an N<sub>2</sub> atmosphere and stirred for 15 min. Then a solution of 2-bromobenzaldehyde (1.05 g, 5.70 mmol) in dry THF (5 ml)

was added and the mixture was allowed to stir for an additional 1 h. After completion of the reaction (monitored by TLC), the mixture was poured over crushed ice (100 g) containing concentrated HCl (1 ml). The solid formed was filtered and washed with methanol to afford ethenylindole **III** as a bright-yellow solid (yield: 1.72 g, 71%). M.p. = 419–421 K.

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 6. All C-bound H atoms were positioned geometrically and constrained to ride on their parent atoms with C–H = 0.93–0.97 Å with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C–methyl) and 1.2*U*<sub>eq</sub>(C) for other H atoms.

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## supporting information

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## The crystal structures and Hirshfeld surface analysis of three new bromo-substituted 3-methyl-1-(phenylsulfonyl)-1*H*-indole derivatives

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### Computing details

#### 2-(Bromomethyl)-3-methyl-1-(phenylsulfonyl)-1*H*-indole (I)

##### Crystal data

C<sub>16</sub>H<sub>14</sub>BrNO<sub>2</sub>S

*M<sub>r</sub>* = 364.25

Monoclinic, *P*2<sub>1</sub>/*c*

*a* = 7.979 (6) Å

*b* = 11.100 (8) Å

*c* = 17.540 (14) Å

β = 99.04 (3)°

*V* = 1534 (2) Å<sup>3</sup>

*Z* = 4

*F*(000) = 736

*D<sub>x</sub>* = 1.577 Mg m<sup>-3</sup>

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 66991 reflections

θ = 1.4–25.0°

μ = 2.82 mm<sup>-1</sup>

*T* = 298 K

Prism, colorless

0.30 × 0.24 × 0.07 mm

##### Data collection

Bruker D8 Venture Diffractometer

Radiation source: micro focus sealed tube

ω and φ scans

Absorption correction: multi-scan

(*SADABS*; Krause *et al.*, 2015)

*T<sub>min</sub>* = 0.589, *T<sub>max</sub>* = 0.753

66991 measured reflections

4464 independent reflections

3158 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.049

θ<sub>max</sub> = 30.0°, θ<sub>min</sub> = 3.2°

*h* = -11→10

*k* = -15→15

*l* = -24→24

##### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.046

*wR*(*F*<sup>2</sup>) = 0.118

*S* = 1.10

4464 reflections

191 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/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0434*P*)<sup>2</sup> + 1.2291*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.75 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.80 e Å<sup>-3</sup>

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3530 (3)	0.4783 (2)	0.58255 (14)	0.0345 (5)
C2	0.3824 (3)	0.3757 (2)	0.62843 (16)	0.0439 (6)
H2	0.446932	0.378932	0.677377	0.053*
C3	0.3113 (4)	0.2684 (2)	0.59810 (18)	0.0513 (7)
H3	0.328360	0.198413	0.627406	0.062*
C4	0.2149 (4)	0.2635 (3)	0.5247 (2)	0.0570 (7)
H4	0.168902	0.190393	0.505784	0.068*
C5	0.1868 (4)	0.3654 (3)	0.47978 (18)	0.0526 (7)
H5	0.122660	0.361549	0.430761	0.063*
C6	0.2562 (3)	0.4750 (2)	0.50893 (14)	0.0387 (5)
C7	0.2515 (3)	0.5952 (2)	0.47726 (15)	0.0428 (6)
C8	0.3405 (3)	0.6691 (2)	0.53034 (14)	0.0398 (5)
C9	0.2921 (3)	0.6242 (2)	0.73345 (14)	0.0385 (5)
C10	0.2971 (4)	0.5343 (3)	0.78836 (17)	0.0537 (7)
H10	0.395387	0.489561	0.803309	0.064*
C11	0.1513 (5)	0.5123 (3)	0.8207 (2)	0.0656 (9)
H11	0.151977	0.452309	0.857811	0.079*
C12	0.0065 (4)	0.5786 (3)	0.7982 (2)	0.0620 (8)
H12	-0.090984	0.562026	0.819260	0.074*
C13	0.0053 (4)	0.6692 (3)	0.74490 (18)	0.0585 (8)
H13	-0.092489	0.714723	0.730838	0.070*
C14	0.1477 (3)	0.6933 (3)	0.71194 (15)	0.0482 (6)
H14	0.146765	0.754810	0.675899	0.058*
C15	0.3845 (4)	0.7966 (2)	0.51928 (19)	0.0540 (7)
H15A	0.397273	0.808599	0.465716	0.065*
H15B	0.493150	0.813659	0.550710	0.065*
C16	0.1665 (5)	0.6285 (3)	0.39759 (17)	0.0642 (9)
H16A	0.177941	0.713609	0.389959	0.096*
H16B	0.048275	0.607924	0.391753	0.096*
H16C	0.218751	0.585444	0.360103	0.096*
N1	0.4082 (3)	0.59886 (17)	0.59670 (12)	0.0369 (4)
O1	0.5039 (3)	0.77321 (19)	0.68162 (13)	0.0614 (6)
O2	0.6017 (2)	0.5675 (2)	0.72121 (13)	0.0596 (6)
S1	0.47047 (8)	0.64724 (6)	0.68698 (4)	0.04217 (16)
Br1	0.21361 (5)	0.91337 (3)	0.54636 (2)	0.07195 (15)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0357 (11)	0.0336 (11)	0.0354 (12)	-0.0001 (9)	0.0087 (9)	-0.0030 (9)
C2	0.0492 (14)	0.0417 (13)	0.0413 (13)	0.0019 (11)	0.0085 (11)	0.0015 (11)
C3	0.0574 (17)	0.0350 (13)	0.0632 (18)	0.0002 (12)	0.0148 (14)	0.0037 (12)
C4	0.0605 (18)	0.0385 (14)	0.071 (2)	-0.0082 (13)	0.0083 (15)	-0.0132 (14)
C5	0.0523 (16)	0.0507 (16)	0.0517 (16)	0.0003 (13)	-0.0014 (13)	-0.0157 (13)
C6	0.0379 (12)	0.0400 (13)	0.0385 (13)	0.0043 (10)	0.0069 (10)	-0.0064 (10)
C7	0.0480 (14)	0.0442 (14)	0.0369 (12)	0.0126 (11)	0.0086 (11)	-0.0006 (11)
C8	0.0486 (14)	0.0343 (12)	0.0395 (13)	0.0082 (10)	0.0162 (11)	0.0029 (10)
C9	0.0442 (13)	0.0389 (12)	0.0319 (11)	-0.0030 (10)	0.0042 (10)	-0.0091 (10)
C10	0.0686 (19)	0.0485 (16)	0.0460 (15)	0.0103 (14)	0.0153 (14)	0.0029 (13)
C11	0.092 (3)	0.0532 (18)	0.0582 (19)	-0.0030 (17)	0.0335 (18)	0.0052 (15)
C12	0.0607 (19)	0.074 (2)	0.0563 (18)	-0.0052 (16)	0.0254 (15)	-0.0081 (16)
C13	0.0460 (15)	0.077 (2)	0.0536 (17)	0.0048 (15)	0.0101 (13)	-0.0018 (16)
C14	0.0479 (14)	0.0577 (17)	0.0382 (13)	0.0023 (13)	0.0042 (11)	0.0022 (12)
C15	0.0698 (19)	0.0387 (14)	0.0599 (18)	0.0037 (13)	0.0303 (15)	0.0048 (12)
C16	0.079 (2)	0.070 (2)	0.0418 (15)	0.0249 (18)	0.0027 (14)	0.0042 (15)
N1	0.0430 (11)	0.0327 (10)	0.0356 (10)	-0.0025 (8)	0.0082 (8)	-0.0037 (8)
O1	0.0733 (14)	0.0497 (12)	0.0623 (13)	-0.0260 (11)	0.0137 (11)	-0.0174 (10)
O2	0.0384 (10)	0.0789 (15)	0.0577 (12)	0.0025 (10)	-0.0047 (9)	-0.0067 (11)
S1	0.0380 (3)	0.0465 (4)	0.0413 (3)	-0.0093 (3)	0.0036 (2)	-0.0100 (3)
Br1	0.1035 (3)	0.03893 (17)	0.0794 (3)	0.01814 (16)	0.0331 (2)	0.00174 (15)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

C1—C2	1.393 (4)	C10—C11	1.394 (5)
C1—C6	1.397 (4)	C10—H10	0.9300
C1—N1	1.419 (3)	C11—C12	1.374 (5)
C2—C3	1.388 (4)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.372 (5)
C3—C4	1.393 (5)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.379 (4)
C4—C5	1.377 (5)	C13—H13	0.9300
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.399 (4)	C15—Br1	1.992 (3)
C5—H5	0.9300	C15—H15A	0.9700
C6—C7	1.444 (4)	C15—H15B	0.9700
C7—C8	1.355 (4)	C16—H16A	0.9600
C7—C16	1.501 (4)	C16—H16B	0.9600
C8—N1	1.434 (3)	C16—H16C	0.9600
C8—C15	1.478 (4)	N1—S1	1.672 (2)
C9—C10	1.384 (4)	O1—S1	1.429 (2)
C9—C14	1.386 (4)	O2—S1	1.430 (2)
C9—S1	1.766 (3)		
C2—C1—C6	122.0 (2)	C10—C11—H11	119.8

C2—C1—N1	130.6 (2)	C13—C12—C11	120.2 (3)
C6—C1—N1	107.3 (2)	C13—C12—H12	119.9
C3—C2—C1	117.3 (3)	C11—C12—H12	119.9
C3—C2—H2	121.4	C12—C13—C14	120.6 (3)
C1—C2—H2	121.4	C12—C13—H13	119.7
C2—C3—C4	121.4 (3)	C14—C13—H13	119.7
C2—C3—H3	119.3	C13—C14—C9	118.9 (3)
C4—C3—H3	119.3	C13—C14—H14	120.6
C5—C4—C3	120.9 (3)	C9—C14—H14	120.6
C5—C4—H4	119.6	C8—C15—Br1	113.97 (19)
C3—C4—H4	119.6	C8—C15—H15A	108.8
C4—C5—C6	119.1 (3)	Br1—C15—H15A	108.8
C4—C5—H5	120.5	C8—C15—H15B	108.8
C6—C5—H5	120.5	Br1—C15—H15B	108.8
C1—C6—C5	119.4 (2)	H15A—C15—H15B	107.7
C1—C6—C7	108.0 (2)	C7—C16—H16A	109.5
C5—C6—C7	132.7 (2)	C7—C16—H16B	109.5
C8—C7—C6	108.4 (2)	H16A—C16—H16B	109.5
C8—C7—C16	127.0 (3)	C7—C16—H16C	109.5
C6—C7—C16	124.5 (3)	H16A—C16—H16C	109.5
C7—C8—N1	108.6 (2)	H16B—C16—H16C	109.5
C7—C8—C15	126.8 (3)	C1—N1—C8	107.7 (2)
N1—C8—C15	124.0 (3)	C1—N1—S1	120.44 (16)
C10—C9—C14	121.4 (3)	C8—N1—S1	127.74 (17)
C10—C9—S1	119.2 (2)	O1—S1—O2	120.11 (14)
C14—C9—S1	119.4 (2)	O1—S1—N1	106.42 (12)
C9—C10—C11	118.4 (3)	O2—S1—N1	106.72 (12)
C9—C10—H10	120.8	O1—S1—C9	110.12 (13)
C11—C10—H10	120.8	O2—S1—C9	107.87 (14)
C12—C11—C10	120.5 (3)	N1—S1—C9	104.46 (12)
C12—C11—H11	119.8		
C6—C1—C2—C3	0.0 (4)	C10—C9—C14—C13	-1.6 (4)
N1—C1—C2—C3	-179.5 (2)	S1—C9—C14—C13	175.7 (2)
C1—C2—C3—C4	0.2 (4)	C7—C8—C15—Br1	90.8 (3)
C2—C3—C4—C5	-0.1 (5)	N1—C8—C15—Br1	-98.9 (3)
C3—C4—C5—C6	-0.2 (5)	C2—C1—N1—C8	-179.5 (2)
C2—C1—C6—C5	-0.3 (4)	C6—C1—N1—C8	0.8 (3)
N1—C1—C6—C5	179.3 (2)	C2—C1—N1—S1	-20.7 (4)
C2—C1—C6—C7	-179.7 (2)	C6—C1—N1—S1	159.66 (17)
N1—C1—C6—C7	-0.1 (3)	C7—C8—N1—C1	-1.3 (3)
C4—C5—C6—C1	0.4 (4)	C15—C8—N1—C1	-173.2 (2)
C4—C5—C6—C7	179.6 (3)	C7—C8—N1—S1	-158.14 (19)
C1—C6—C7—C8	-0.8 (3)	C15—C8—N1—S1	30.0 (3)
C5—C6—C7—C8	179.9 (3)	C1—N1—S1—O1	-175.28 (19)
C1—C6—C7—C16	177.2 (3)	C8—N1—S1—O1	-21.1 (2)
C5—C6—C7—C16	-2.1 (5)	C1—N1—S1—O2	55.3 (2)
C6—C7—C8—N1	1.3 (3)	C8—N1—S1—O2	-150.5 (2)

C16—C7—C8—N1	-176.6 (3)	C1—N1—S1—C9	-58.8 (2)
C6—C7—C8—C15	172.8 (2)	C8—N1—S1—C9	95.4 (2)
C16—C7—C8—C15	-5.0 (5)	C10—C9—S1—O1	-136.9 (2)
C14—C9—C10—C11	1.5 (4)	C14—C9—S1—O1	45.7 (2)
S1—C9—C10—C11	-175.9 (2)	C10—C9—S1—O2	-4.1 (3)
C9—C10—C11—C12	0.1 (5)	C14—C9—S1—O2	178.5 (2)
C10—C11—C12—C13	-1.5 (5)	C10—C9—S1—N1	109.2 (2)
C11—C12—C13—C14	1.4 (5)	C14—C9—S1—N1	-68.2 (2)
C12—C13—C14—C9	0.2 (5)		

## Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O2	0.93	2.49	3.057 (4)	120
C2—H2...O1 <sup>i</sup>	0.93	2.71	3.503 (4)	144
C10—H10...O1 <sup>i</sup>	0.93	2.53	3.306 (4)	141
C12—H12...O2 <sup>ii</sup>	0.93	2.77	3.302 (5)	118
C13—H13...O2 <sup>ii</sup>	0.93	2.92	3.376 (4)	112
C16—H16C...O2 <sup>iii</sup>	0.96	2.76	3.702 (4)	168
C4—H4...Br1 <sup>iv</sup>	0.93	3.16	3.905 (4)	138
C12—H12...Br1 <sup>v</sup>	0.93	3.16	3.922 (4)	141
C14—H14...Br1	0.93	2.99	3.894 (4)	165
C16—H16A...Cg(C9—C14) <sup>vi</sup>	0.96	2.97	3.765 (4)	142
C16—H16B...Cg(C1—C6) <sup>vii</sup>	0.96	2.97	3.823 (5)	149

Symmetry codes: (i)  $-x+1, y-1/2, -z+3/2$ ; (ii)  $x-1, y, z$ ; (iii)  $-x+1, -y+1, -z+1$ ; (iv)  $x, y-1, z$ ; (v)  $-x, y-1/2, -z+3/2$ ; (vi)  $x, -y+3/2, z-1/2$ ; (vii)  $-x, -y+1, -z+1$ .

2-[(*E*)-2-(2-Bromo-5-methoxyphenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole (II)

## Crystal data

C<sub>24</sub>H<sub>20</sub>BrNO<sub>3</sub>S*M<sub>r</sub>* = 482.38Monoclinic, *P*2<sub>1</sub>/*c**a* = 8.4252 (9) Å*b* = 28.669 (3) Å*c* = 8.9462 (11) Å

β = 95.445 (4)°

*V* = 2151.1 (4) Å<sup>3</sup>*Z* = 4*F*(000) = 984*D<sub>x</sub>* = 1.489 Mg m<sup>-3</sup>Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 52480 reflections

θ = 1.4–25.0°

μ = 2.03 mm<sup>-1</sup>*T* = 298 K

Solid, yellow

0.25 × 0.20 × 0.13 mm

## Data collection

Bruker D8 Venture Diffractometer

Radiation source: micro focus sealed tube

ω and φ scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)*T<sub>min</sub>* = 0.555, *T<sub>max</sub>* = 0.745

52479 measured reflections

5296 independent reflections

3905 reflections with *I* > 2σ(*I*)*R<sub>int</sub>* = 0.077θ<sub>max</sub> = 28.3°, θ<sub>min</sub> = 3.3°*h* = -11→11*k* = -38→38*l* = -11→11

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.099$   
 $S = 1.03$   
 5296 reflections  
 272 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.0393P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6561 (3)	0.48550 (8)	0.3470 (2)	0.0469 (5)
C2	0.6281 (3)	0.50829 (10)	0.2093 (3)	0.0614 (6)
H2	0.568729	0.494387	0.128332	0.074*
C3	0.6923 (4)	0.55236 (11)	0.1981 (3)	0.0717 (8)
H3	0.676266	0.568262	0.107279	0.086*
C4	0.7791 (4)	0.57337 (10)	0.3175 (4)	0.0742 (8)
H4	0.820363	0.603085	0.305664	0.089*
C5	0.8062 (3)	0.55132 (9)	0.4542 (3)	0.0643 (7)
H5	0.863821	0.565906	0.534811	0.077*
C6	0.7446 (3)	0.50632 (8)	0.4686 (2)	0.0473 (5)
C7	0.7513 (3)	0.47458 (8)	0.5935 (2)	0.0461 (5)
C8	0.6716 (2)	0.43516 (7)	0.5475 (2)	0.0421 (4)
C9	0.7837 (3)	0.38292 (8)	0.2424 (3)	0.0489 (5)
C10	0.8684 (3)	0.35109 (10)	0.3337 (3)	0.0673 (7)
H10	0.820424	0.335580	0.408902	0.081*
C11	1.0261 (4)	0.34260 (13)	0.3116 (4)	0.0860 (10)
H11	1.084868	0.321232	0.372357	0.103*
C12	1.0964 (4)	0.36561 (13)	0.2001 (5)	0.0861 (10)
H12	1.202336	0.359691	0.185423	0.103*
C13	1.0103 (4)	0.39724 (12)	0.1108 (4)	0.0805 (9)
H13	1.058787	0.412993	0.036429	0.097*
C14	0.8539 (4)	0.40589 (10)	0.1299 (3)	0.0643 (7)
H14	0.795426	0.426986	0.067855	0.077*
C15	0.6383 (3)	0.39387 (8)	0.6346 (2)	0.0444 (5)
H15	0.536056	0.381323	0.623013	0.053*
C16	0.7478 (3)	0.37332 (7)	0.7300 (2)	0.0438 (5)
H16	0.851979	0.384173	0.732095	0.053*
C17	0.7170 (2)	0.33490 (7)	0.8319 (2)	0.0400 (4)

C18	0.5683 (3)	0.32918 (7)	0.8844 (2)	0.0438 (5)
H18	0.486448	0.349562	0.851587	0.053*
C19	0.5381 (3)	0.29388 (8)	0.9845 (3)	0.0490 (5)
C20	0.6587 (3)	0.26380 (9)	1.0366 (3)	0.0599 (6)
H20	0.639903	0.240384	1.104648	0.072*
C21	0.8074 (3)	0.26891 (8)	0.9866 (3)	0.0580 (6)
H21	0.889518	0.248965	1.022176	0.070*
C22	0.8361 (3)	0.30307 (7)	0.8848 (3)	0.0455 (5)
C23	0.8223 (4)	0.48672 (10)	0.7485 (3)	0.0681 (7)
H23A	0.791508	0.463736	0.818252	0.102*
H23B	0.784469	0.516817	0.776049	0.102*
H23C	0.936409	0.487396	0.750554	0.102*
C24	0.3489 (4)	0.25800 (13)	1.1295 (4)	0.0971 (12)
H24A	0.238662	0.260695	1.147390	0.146*
H24B	0.368142	0.227541	1.090527	0.146*
H24C	0.414581	0.262561	1.222022	0.146*
N1	0.6044 (2)	0.44108 (6)	0.39484 (19)	0.0449 (4)
O1	0.5205 (2)	0.35818 (6)	0.3525 (2)	0.0635 (5)
O2	0.5020 (2)	0.41358 (7)	0.1409 (2)	0.0722 (5)
O3	0.3861 (2)	0.29237 (7)	1.0239 (2)	0.0704 (5)
S1	0.58589 (7)	0.39595 (2)	0.27518 (6)	0.05060 (15)
Br1	1.04254 (3)	0.30608 (2)	0.81730 (3)	0.06603 (11)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0452 (11)	0.0509 (12)	0.0454 (12)	0.0121 (9)	0.0092 (9)	0.0073 (10)
C2	0.0653 (16)	0.0700 (16)	0.0493 (13)	0.0168 (13)	0.0076 (11)	0.0139 (12)
C3	0.0784 (19)	0.0731 (18)	0.0660 (17)	0.0233 (15)	0.0194 (15)	0.0311 (15)
C4	0.0778 (19)	0.0526 (15)	0.096 (2)	0.0088 (14)	0.0262 (17)	0.0275 (15)
C5	0.0702 (17)	0.0495 (14)	0.0740 (17)	-0.0018 (12)	0.0115 (14)	0.0052 (13)
C6	0.0507 (12)	0.0435 (11)	0.0487 (12)	0.0066 (9)	0.0099 (10)	0.0047 (10)
C7	0.0494 (12)	0.0470 (12)	0.0419 (11)	0.0026 (9)	0.0044 (9)	0.0013 (9)
C8	0.0423 (11)	0.0477 (11)	0.0367 (10)	0.0055 (9)	0.0060 (8)	0.0032 (9)
C9	0.0481 (12)	0.0526 (13)	0.0459 (12)	-0.0051 (10)	0.0036 (10)	-0.0127 (10)
C10	0.0614 (16)	0.0698 (17)	0.0714 (17)	0.0112 (13)	0.0100 (13)	-0.0006 (14)
C11	0.0666 (19)	0.090 (2)	0.100 (2)	0.0239 (17)	0.0004 (18)	-0.0126 (19)
C12	0.0518 (16)	0.096 (2)	0.112 (3)	-0.0075 (16)	0.0195 (18)	-0.048 (2)
C13	0.082 (2)	0.080 (2)	0.086 (2)	-0.0191 (17)	0.0400 (18)	-0.0266 (18)
C14	0.0738 (17)	0.0673 (16)	0.0539 (14)	-0.0036 (13)	0.0167 (13)	-0.0091 (12)
C15	0.0440 (11)	0.0474 (12)	0.0425 (11)	-0.0010 (9)	0.0072 (9)	0.0013 (9)
C16	0.0408 (11)	0.0435 (11)	0.0477 (12)	0.0008 (9)	0.0069 (9)	-0.0008 (9)
C17	0.0424 (10)	0.0366 (10)	0.0399 (10)	0.0003 (8)	-0.0020 (8)	-0.0027 (8)
C18	0.0431 (11)	0.0431 (11)	0.0441 (11)	0.0017 (9)	-0.0021 (9)	0.0038 (9)
C19	0.0469 (12)	0.0514 (12)	0.0471 (12)	-0.0059 (10)	-0.0028 (10)	0.0076 (10)
C20	0.0614 (15)	0.0531 (14)	0.0631 (15)	-0.0030 (11)	-0.0060 (12)	0.0201 (12)
C21	0.0559 (14)	0.0472 (13)	0.0683 (16)	0.0097 (11)	-0.0081 (12)	0.0115 (12)
C22	0.0422 (11)	0.0425 (11)	0.0505 (12)	0.0036 (9)	-0.0022 (9)	-0.0057 (9)



C23	0.093 (2)	0.0577 (15)	0.0510 (14)	-0.0049 (14)	-0.0060 (14)	-0.0038 (12)
C24	0.079 (2)	0.110 (3)	0.106 (3)	-0.0124 (19)	0.0235 (19)	0.053 (2)
N1	0.0454 (9)	0.0490 (10)	0.0399 (9)	0.0047 (8)	0.0018 (7)	0.0024 (8)
O1	0.0581 (10)	0.0660 (11)	0.0666 (11)	-0.0193 (8)	0.0066 (8)	-0.0049 (9)
O2	0.0665 (11)	0.0939 (14)	0.0512 (10)	0.0062 (10)	-0.0195 (8)	-0.0042 (9)
O3	0.0510 (10)	0.0845 (13)	0.0760 (12)	-0.0058 (9)	0.0077 (9)	0.0337 (10)
S1	0.0441 (3)	0.0620 (4)	0.0443 (3)	-0.0022 (3)	-0.0033 (2)	-0.0053 (3)
Br1	0.04735 (15)	0.06198 (17)	0.0897 (2)	0.01104 (11)	0.01150 (13)	-0.00450 (14)

*Geometric parameters (Å, °)*

C1—C6	1.393 (3)	C14—H14	0.9300
C1—C2	1.395 (3)	C15—C16	1.333 (3)
C1—N1	1.425 (3)	C15—H15	0.9300
C2—C3	1.382 (4)	C16—C17	1.469 (3)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.375 (4)	C17—C18	1.389 (3)
C3—H3	0.9300	C17—C22	1.405 (3)
C4—C5	1.376 (4)	C18—C19	1.391 (3)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.401 (3)	C19—O3	1.360 (3)
C5—H5	0.9300	C19—C20	1.380 (3)
C6—C7	1.438 (3)	C20—C21	1.377 (4)
C7—C8	1.358 (3)	C20—H20	0.9300
C7—C23	1.498 (3)	C21—C22	1.374 (3)
C8—N1	1.438 (3)	C21—H21	0.9300
C8—C15	1.459 (3)	C22—Br1	1.896 (2)
C9—C10	1.378 (4)	C23—H23A	0.9600
C9—C14	1.382 (3)	C23—H23B	0.9600
C9—S1	1.759 (2)	C23—H23C	0.9600
C10—C11	1.383 (4)	C24—O3	1.421 (3)
C10—H10	0.9300	C24—H24A	0.9600
C11—C12	1.376 (5)	C24—H24B	0.9600
C11—H11	0.9300	C24—H24C	0.9600
C12—C13	1.370 (5)	N1—S1	1.6770 (19)
C12—H12	0.9300	O1—S1	1.4237 (19)
C13—C14	1.368 (4)	O2—S1	1.4269 (18)
C13—H13	0.9300		
C6—C1—C2	121.5 (2)	C8—C15—H15	118.5
C6—C1—N1	107.75 (18)	C15—C16—C17	125.2 (2)
C2—C1—N1	130.7 (2)	C15—C16—H16	117.4
C3—C2—C1	117.2 (3)	C17—C16—H16	117.4
C3—C2—H2	121.4	C18—C17—C22	116.61 (19)
C1—C2—H2	121.4	C18—C17—C16	121.10 (18)
C4—C3—C2	121.8 (2)	C22—C17—C16	122.26 (19)
C4—C3—H3	119.1	C17—C18—C19	122.0 (2)
C2—C3—H3	119.1	C17—C18—H18	119.0

C3—C4—C5	121.4 (3)	C19—C18—H18	119.0
C3—C4—H4	119.3	O3—C19—C20	125.0 (2)
C5—C4—H4	119.3	O3—C19—C18	115.1 (2)
C4—C5—C6	118.3 (3)	C20—C19—C18	119.9 (2)
C4—C5—H5	120.9	C21—C20—C19	119.2 (2)
C6—C5—H5	120.9	C21—C20—H20	120.4
C1—C6—C5	119.8 (2)	C19—C20—H20	120.4
C1—C6—C7	108.3 (2)	C22—C21—C20	120.9 (2)
C5—C6—C7	131.8 (2)	C22—C21—H21	119.5
C8—C7—C6	108.00 (19)	C20—C21—H21	119.5
C8—C7—C23	128.0 (2)	C21—C22—C17	121.4 (2)
C6—C7—C23	123.7 (2)	C21—C22—Br1	117.89 (17)
C7—C8—N1	109.18 (18)	C17—C22—Br1	120.70 (17)
C7—C8—C15	128.9 (2)	C7—C23—H23A	109.5
N1—C8—C15	121.62 (19)	C7—C23—H23B	109.5
C10—C9—C14	120.9 (2)	H23A—C23—H23B	109.5
C10—C9—S1	119.18 (19)	C7—C23—H23C	109.5
C14—C9—S1	119.9 (2)	H23A—C23—H23C	109.5
C9—C10—C11	118.8 (3)	H23B—C23—H23C	109.5
C9—C10—H10	120.6	O3—C24—H24A	109.5
C11—C10—H10	120.6	O3—C24—H24B	109.5
C12—C11—C10	120.3 (3)	H24A—C24—H24B	109.5
C12—C11—H11	119.8	O3—C24—H24C	109.5
C10—C11—H11	119.8	H24A—C24—H24C	109.5
C13—C12—C11	120.0 (3)	H24B—C24—H24C	109.5
C13—C12—H12	120.0	C1—N1—C8	106.63 (17)
C11—C12—H12	120.0	C1—N1—S1	120.69 (15)
C14—C13—C12	120.7 (3)	C8—N1—S1	121.31 (15)
C14—C13—H13	119.7	C19—O3—C24	117.8 (2)
C12—C13—H13	119.7	O1—S1—O2	119.67 (12)
C13—C14—C9	119.3 (3)	O1—S1—N1	107.06 (10)
C13—C14—H14	120.4	O2—S1—N1	105.82 (11)
C9—C14—H14	120.4	O1—S1—C9	109.61 (12)
C16—C15—C8	122.9 (2)	O2—S1—C9	109.65 (12)
C16—C15—H15	118.5	N1—S1—C9	103.78 (10)
C6—C1—C2—C3	0.2 (4)	C17—C18—C19—O3	-179.1 (2)
N1—C1—C2—C3	178.4 (2)	C17—C18—C19—C20	1.2 (4)
C1—C2—C3—C4	-0.6 (4)	O3—C19—C20—C21	179.4 (2)
C2—C3—C4—C5	0.0 (4)	C18—C19—C20—C21	-0.9 (4)
C3—C4—C5—C6	0.8 (4)	C19—C20—C21—C22	-0.7 (4)
C2—C1—C6—C5	0.6 (3)	C20—C21—C22—C17	2.1 (4)
N1—C1—C6—C5	-177.9 (2)	C20—C21—C22—Br1	-177.9 (2)
C2—C1—C6—C7	179.6 (2)	C18—C17—C22—C21	-1.8 (3)
N1—C1—C6—C7	1.0 (2)	C16—C17—C22—C21	176.4 (2)
C4—C5—C6—C1	-1.1 (4)	C18—C17—C22—Br1	178.23 (15)
C4—C5—C6—C7	-179.8 (2)	C16—C17—C22—Br1	-3.6 (3)
C1—C6—C7—C8	1.2 (3)	C6—C1—N1—C8	-2.7 (2)

C5—C6—C7—C8	180.0 (3)	C2—C1—N1—C8	178.9 (2)
C1—C6—C7—C23	-173.6 (2)	C6—C1—N1—S1	-146.59 (16)
C5—C6—C7—C23	5.2 (4)	C2—C1—N1—S1	35.0 (3)
C6—C7—C8—N1	-2.9 (2)	C7—C8—N1—C1	3.5 (2)
C23—C7—C8—N1	171.6 (2)	C15—C8—N1—C1	177.77 (19)
C6—C7—C8—C15	-176.6 (2)	C7—C8—N1—S1	147.12 (16)
C23—C7—C8—C15	-2.1 (4)	C15—C8—N1—S1	-38.6 (3)
C14—C9—C10—C11	0.4 (4)	C20—C19—O3—C24	1.6 (4)
S1—C9—C10—C11	-177.1 (2)	C18—C19—O3—C24	-178.1 (3)
C9—C10—C11—C12	-0.1 (5)	C1—N1—S1—O1	-175.43 (16)
C10—C11—C12—C13	0.3 (5)	C8—N1—S1—O1	45.94 (19)
C11—C12—C13—C14	-0.8 (5)	C1—N1—S1—O2	-46.74 (19)
C12—C13—C14—C9	1.1 (4)	C8—N1—S1—O2	174.62 (17)
C10—C9—C14—C13	-0.9 (4)	C1—N1—S1—C9	68.69 (18)
S1—C9—C14—C13	176.6 (2)	C8—N1—S1—C9	-69.95 (18)
C7—C8—C15—C16	-45.2 (3)	C10—C9—S1—O1	-23.7 (2)
N1—C8—C15—C16	141.7 (2)	C14—C9—S1—O1	158.74 (19)
C8—C15—C16—C17	173.14 (19)	C10—C9—S1—O2	-157.0 (2)
C15—C16—C17—C18	-27.4 (3)	C14—C9—S1—O2	25.5 (2)
C15—C16—C17—C22	154.5 (2)	C10—C9—S1—N1	90.3 (2)
C22—C17—C18—C19	0.2 (3)	C14—C9—S1—N1	-87.2 (2)
C16—C17—C18—C19	-178.1 (2)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O2	0.93	2.39	2.958 (4)	119
C3—H3 $\cdots$ O2 <sup>i</sup>	0.93	2.61	3.448 (3)	150
C24—H24A $\cdots$ Br1 <sup>ii</sup>	0.96	3.03	3.699 (3)	128
C5—H5 $\cdots$ Cg(C9—C14) <sup>iii</sup>	0.93	3.12	4.047 (3)	173
C20—H20 $\cdots$ Cg(C17—C22) <sup>iv</sup>	0.93	3.15	3.978 (2)	149
C23—H23C $\cdots$ Cg(C1—C6) <sup>iii</sup>	0.96	3.11	4.036 (4)	162

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $x-1, -y+1/2, z+1/2$ ; (iii)  $-x+2, -y+1, -z+1$ ; (iv)  $x, -y+1/2, z+1/2$ .2-[(*E*)-2-(2-Bromophenyl)ethenyl]-3-methyl-1-(phenylsulfonyl)-1*H*-indole (III)

## Crystal data

 $C_{23}H_{18}BrNO_2S$  $M_r = 452.35$ Monoclinic,  $P2_1/n$  $a = 12.5530$  (8)  $\text{\AA}$  $b = 8.3533$  (5)  $\text{\AA}$  $c = 19.7698$  (11)  $\text{\AA}$  $\beta = 107.078$  (2) $^\circ$  $V = 1981.6$  (2)  $\text{\AA}^3$  $Z = 4$  $F(000) = 920$  $D_x = 1.516$  Mg  $\text{m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073$   $\text{\AA}$ 

Cell parameters from 50531 reflections

 $\theta = 1.4\text{--}25.0^\circ$  $\mu = 2.20$   $\text{mm}^{-1}$  $T = 298$  K

Prism, yellow

 $0.36 \times 0.31 \times 0.24$  mm

Data collection

Bruker D8 Venture Diffractometer  
 Radiation source: micro focus sealed tube  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan  
 (SADABS; Krause *et al.*, 2015)  
 $T_{\min} = 0.514$ ,  $T_{\max} = 0.745$   
 50531 measured reflections

4293 independent reflections  
 3516 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.058$   
 $\theta_{\max} = 27.0^\circ$ ,  $\theta_{\min} = 2.7^\circ$   
 $h = -16 \rightarrow 16$   
 $k = -10 \rightarrow 10$   
 $l = -25 \rightarrow 25$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.087$   
 $S = 1.10$   
 4293 reflections  
 254 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 1.371P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3845 (2)	0.7169 (3)	0.40613 (15)	0.0514 (6)
C2	0.2805 (2)	0.6430 (4)	0.3796 (2)	0.0725 (9)
H2	0.242636	0.642367	0.331512	0.087*
C3	0.2367 (3)	0.5708 (4)	0.4288 (3)	0.0861 (12)
H3	0.168029	0.519654	0.413097	0.103*
C4	0.2916 (3)	0.5724 (4)	0.5001 (3)	0.0847 (11)
H4	0.258724	0.524019	0.531342	0.102*
C5	0.3941 (3)	0.6443 (4)	0.52611 (19)	0.0691 (9)
H5	0.430809	0.644742	0.574390	0.083*
C6	0.4420 (2)	0.7169 (3)	0.47795 (15)	0.0510 (6)
C7	0.5465 (2)	0.7977 (3)	0.48800 (13)	0.0461 (6)
C8	0.55284 (19)	0.8444 (3)	0.42348 (13)	0.0430 (5)
C9	0.5022 (2)	0.5840 (3)	0.28233 (12)	0.0434 (5)
C10	0.6151 (2)	0.5774 (3)	0.28776 (13)	0.0516 (6)
H10	0.658022	0.670085	0.295131	0.062*
C11	0.6624 (3)	0.4304 (4)	0.28198 (15)	0.0618 (7)
H11	0.737661	0.423945	0.285032	0.074*
C12	0.5984 (3)	0.2933 (3)	0.27172 (14)	0.0627 (8)
H12	0.630690	0.194953	0.267756	0.075*
C13	0.4875 (3)	0.3010 (3)	0.26731 (15)	0.0609 (7)
H13	0.445370	0.207621	0.260770	0.073*

C14	0.4379 (2)	0.4461 (3)	0.27251 (13)	0.0532 (6)
H14	0.362668	0.451289	0.269471	0.064*
C15	0.6425 (2)	0.9296 (3)	0.40580 (12)	0.0443 (5)
H15	0.625141	1.018220	0.376123	0.053*
C16	0.7487 (2)	0.8842 (3)	0.43088 (12)	0.0425 (5)
H16	0.763379	0.793865	0.459639	0.051*
C17	0.84434 (19)	0.9639 (3)	0.41719 (11)	0.0393 (5)
C18	0.8460 (2)	1.1291 (3)	0.40596 (13)	0.0495 (6)
H18	0.784735	1.190395	0.407169	0.059*
C19	0.9364 (3)	1.2033 (3)	0.39313 (14)	0.0572 (7)
H19	0.934596	1.312866	0.384518	0.069*
C20	1.0296 (2)	1.1155 (3)	0.39303 (13)	0.0542 (7)
H20	1.091088	1.166316	0.385527	0.065*
C21	1.0315 (2)	0.9525 (3)	0.40404 (13)	0.0481 (6)
H21	1.093843	0.892468	0.403982	0.058*
C22	0.93913 (19)	0.8795 (3)	0.41520 (12)	0.0402 (5)
C23	0.6286 (3)	0.8304 (4)	0.55857 (14)	0.0608 (7)
H23A	0.670017	0.734729	0.575877	0.091*
H23B	0.589586	0.863969	0.591254	0.091*
H23C	0.678808	0.913412	0.553866	0.091*
N1	0.45078 (16)	0.8027 (2)	0.37072 (11)	0.0471 (5)
O1	0.50537 (19)	0.8925 (2)	0.26566 (10)	0.0640 (5)
O2	0.32416 (17)	0.7603 (3)	0.24957 (11)	0.0761 (6)
S1	0.44041 (6)	0.77168 (8)	0.28558 (3)	0.05103 (17)
Br1	0.94200 (2)	0.65291 (3)	0.42493 (2)	0.06143 (11)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0422 (13)	0.0425 (13)	0.0753 (18)	0.0112 (11)	0.0262 (13)	-0.0021 (12)
C2	0.0454 (15)	0.0663 (19)	0.107 (3)	0.0057 (14)	0.0239 (16)	-0.0137 (18)
C3	0.0554 (19)	0.062 (2)	0.160 (4)	-0.0014 (16)	0.061 (2)	-0.016 (2)
C4	0.089 (3)	0.058 (2)	0.138 (3)	0.0023 (18)	0.081 (3)	-0.005 (2)
C5	0.083 (2)	0.0539 (17)	0.091 (2)	0.0117 (16)	0.0584 (19)	0.0018 (15)
C6	0.0539 (15)	0.0407 (13)	0.0676 (17)	0.0137 (11)	0.0325 (13)	-0.0012 (12)
C7	0.0487 (14)	0.0398 (12)	0.0535 (14)	0.0145 (10)	0.0210 (11)	-0.0012 (11)
C8	0.0400 (12)	0.0379 (12)	0.0511 (13)	0.0111 (10)	0.0132 (10)	-0.0019 (10)
C9	0.0505 (14)	0.0375 (12)	0.0391 (12)	0.0021 (10)	0.0084 (10)	0.0030 (10)
C10	0.0521 (15)	0.0474 (14)	0.0529 (14)	-0.0001 (12)	0.0119 (12)	-0.0011 (12)
C11	0.0604 (17)	0.0616 (18)	0.0611 (17)	0.0177 (14)	0.0144 (13)	0.0008 (14)
C12	0.089 (2)	0.0433 (14)	0.0501 (15)	0.0187 (15)	0.0120 (15)	0.0001 (12)
C13	0.082 (2)	0.0415 (14)	0.0544 (16)	-0.0062 (14)	0.0129 (14)	-0.0009 (12)
C14	0.0561 (15)	0.0474 (15)	0.0535 (15)	-0.0034 (12)	0.0121 (12)	0.0005 (12)
C15	0.0483 (13)	0.0368 (12)	0.0478 (13)	0.0047 (10)	0.0145 (11)	0.0008 (10)
C16	0.0476 (13)	0.0362 (12)	0.0466 (13)	0.0064 (10)	0.0184 (11)	0.0002 (10)
C17	0.0448 (12)	0.0352 (11)	0.0375 (11)	0.0030 (9)	0.0117 (10)	-0.0026 (9)
C18	0.0584 (15)	0.0349 (12)	0.0540 (14)	0.0069 (11)	0.0148 (12)	-0.0014 (10)
C19	0.0750 (19)	0.0367 (13)	0.0567 (16)	-0.0078 (13)	0.0143 (14)	0.0024 (12)

C20	0.0537 (15)	0.0590 (17)	0.0484 (14)	-0.0158 (13)	0.0125 (12)	0.0007 (12)
C21	0.0423 (13)	0.0546 (15)	0.0479 (13)	0.0003 (11)	0.0139 (11)	-0.0029 (11)
C22	0.0458 (12)	0.0322 (11)	0.0419 (12)	0.0032 (9)	0.0115 (10)	-0.0017 (9)
C23	0.0679 (18)	0.0654 (18)	0.0511 (15)	0.0178 (14)	0.0204 (13)	-0.0022 (13)
N1	0.0404 (11)	0.0441 (11)	0.0564 (12)	0.0075 (9)	0.0134 (9)	-0.0016 (9)
O1	0.0944 (15)	0.0394 (10)	0.0564 (11)	0.0035 (10)	0.0194 (10)	0.0085 (8)
O2	0.0572 (12)	0.0791 (15)	0.0734 (13)	0.0209 (11)	-0.0100 (10)	-0.0017 (11)
S1	0.0548 (4)	0.0413 (3)	0.0503 (3)	0.0116 (3)	0.0049 (3)	0.0037 (3)
Br1	0.05484 (17)	0.03621 (14)	0.0976 (2)	0.00739 (11)	0.02920 (15)	-0.00128 (13)

*Geometric parameters (Å, °)*

C1—C6	1.391 (4)	C13—C14	1.380 (4)
C1—C2	1.399 (4)	C13—H13	0.9300
C1—N1	1.428 (3)	C14—H14	0.9300
C2—C3	1.388 (5)	C15—C16	1.333 (3)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.374 (5)	C16—C17	1.466 (3)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.376 (5)	C17—C22	1.394 (3)
C4—H4	0.9300	C17—C18	1.399 (3)
C5—C6	1.404 (4)	C18—C19	1.381 (4)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.437 (4)	C19—C20	1.381 (4)
C7—C8	1.358 (3)	C19—H19	0.9300
C7—C23	1.496 (4)	C20—C21	1.378 (4)
C8—N1	1.437 (3)	C20—H20	0.9300
C8—C15	1.458 (3)	C21—C22	1.383 (3)
C9—C14	1.387 (4)	C21—H21	0.9300
C9—C10	1.390 (4)	C22—Br1	1.902 (2)
C9—S1	1.759 (2)	C23—H23A	0.9600
C10—C11	1.383 (4)	C23—H23B	0.9600
C10—H10	0.9300	C23—H23C	0.9600
C11—C12	1.379 (4)	N1—S1	1.670 (2)
C11—H11	0.9300	O1—S1	1.424 (2)
C12—C13	1.370 (4)	O2—S1	1.427 (2)
C12—H12	0.9300		
C6—C1—C2	122.0 (3)	C9—C14—H14	120.6
C6—C1—N1	107.3 (2)	C16—C15—C8	122.0 (2)
C2—C1—N1	130.7 (3)	C16—C15—H15	119.0
C3—C2—C1	116.5 (3)	C8—C15—H15	119.0
C3—C2—H2	121.7	C15—C16—C17	125.8 (2)
C1—C2—H2	121.7	C15—C16—H16	117.1
C4—C3—C2	122.1 (3)	C17—C16—H16	117.1
C4—C3—H3	118.9	C22—C17—C18	116.2 (2)
C2—C3—H3	118.9	C22—C17—C16	121.9 (2)
C3—C4—C5	121.3 (3)	C18—C17—C16	121.9 (2)

C3—C4—H4	119.3	C19—C18—C17	121.6 (2)
C5—C4—H4	119.3	C19—C18—H18	119.2
C4—C5—C6	118.3 (3)	C17—C18—H18	119.2
C4—C5—H5	120.8	C18—C19—C20	120.3 (2)
C6—C5—H5	120.8	C18—C19—H19	119.9
C1—C6—C5	119.6 (3)	C20—C19—H19	119.9
C1—C6—C7	108.7 (2)	C21—C20—C19	120.0 (3)
C5—C6—C7	131.7 (3)	C21—C20—H20	120.0
C8—C7—C6	107.9 (2)	C19—C20—H20	120.0
C8—C7—C23	127.5 (3)	C20—C21—C22	119.0 (2)
C6—C7—C23	124.4 (2)	C20—C21—H21	120.5
C7—C8—N1	109.1 (2)	C22—C21—H21	120.5
C7—C8—C15	128.9 (2)	C21—C22—C17	123.0 (2)
N1—C8—C15	122.0 (2)	C21—C22—Br1	117.57 (18)
C14—C9—C10	121.0 (2)	C17—C22—Br1	119.44 (17)
C14—C9—S1	120.0 (2)	C7—C23—H23A	109.5
C10—C9—S1	118.91 (19)	C7—C23—H23B	109.5
C11—C10—C9	118.8 (3)	H23A—C23—H23B	109.5
C11—C10—H10	120.6	C7—C23—H23C	109.5
C9—C10—H10	120.6	H23A—C23—H23C	109.5
C12—C11—C10	120.2 (3)	H23B—C23—H23C	109.5
C12—C11—H11	119.9	C1—N1—C8	106.8 (2)
C10—C11—H11	119.9	C1—N1—S1	122.15 (18)
C13—C12—C11	120.5 (3)	C8—N1—S1	123.93 (17)
C13—C12—H12	119.7	O1—S1—O2	119.60 (13)
C11—C12—H12	119.7	O1—S1—N1	106.70 (11)
C12—C13—C14	120.5 (3)	O2—S1—N1	106.19 (12)
C12—C13—H13	119.7	O1—S1—C9	109.10 (12)
C14—C13—H13	119.7	O2—S1—C9	108.67 (13)
C13—C14—C9	118.9 (3)	N1—S1—C9	105.70 (10)
C13—C14—H14	120.6		
C6—C1—C2—C3	0.6 (4)	C22—C17—C18—C19	0.5 (4)
N1—C1—C2—C3	-178.8 (3)	C16—C17—C18—C19	180.0 (2)
C1—C2—C3—C4	0.6 (5)	C17—C18—C19—C20	-1.8 (4)
C2—C3—C4—C5	-1.0 (5)	C18—C19—C20—C21	1.6 (4)
C3—C4—C5—C6	0.1 (5)	C19—C20—C21—C22	-0.1 (4)
C2—C1—C6—C5	-1.5 (4)	C20—C21—C22—C17	-1.3 (4)
N1—C1—C6—C5	178.1 (2)	C20—C21—C22—Br1	176.59 (19)
C2—C1—C6—C7	178.4 (2)	C18—C17—C22—C21	1.1 (3)
N1—C1—C6—C7	-2.0 (3)	C16—C17—C22—C21	-178.4 (2)
C4—C5—C6—C1	1.1 (4)	C18—C17—C22—Br1	-176.75 (17)
C4—C5—C6—C7	-178.8 (3)	C16—C17—C22—Br1	3.7 (3)
C1—C6—C7—C8	-0.6 (3)	C6—C1—N1—C8	3.7 (2)
C5—C6—C7—C8	179.3 (3)	C2—C1—N1—C8	-176.8 (3)
C1—C6—C7—C23	176.2 (2)	C6—C1—N1—S1	155.22 (17)
C5—C6—C7—C23	-3.8 (4)	C2—C1—N1—S1	-25.3 (4)
C6—C7—C8—N1	3.0 (3)	C7—C8—N1—C1	-4.2 (2)

C23—C7—C8—N1	-173.7 (2)	C15—C8—N1—C1	178.2 (2)
C6—C7—C8—C15	-179.6 (2)	C7—C8—N1—S1	-155.05 (17)
C23—C7—C8—C15	3.7 (4)	C15—C8—N1—S1	27.3 (3)
C14—C9—C10—C11	1.1 (4)	C1—N1—S1—O1	171.57 (19)
S1—C9—C10—C11	-177.1 (2)	C8—N1—S1—O1	-41.8 (2)
C9—C10—C11—C12	-0.6 (4)	C1—N1—S1—O2	42.9 (2)
C10—C11—C12—C13	-0.2 (4)	C8—N1—S1—O2	-170.45 (19)
C11—C12—C13—C14	0.5 (4)	C1—N1—S1—C9	-72.4 (2)
C12—C13—C14—C9	-0.1 (4)	C8—N1—S1—C9	74.2 (2)
C10—C9—C14—C13	-0.7 (4)	C14—C9—S1—O1	-155.3 (2)
S1—C9—C14—C13	177.4 (2)	C10—C9—S1—O1	22.9 (2)
C7—C8—C15—C16	48.7 (4)	C14—C9—S1—O2	-23.3 (2)
N1—C8—C15—C16	-134.1 (2)	C10—C9—S1—O2	154.9 (2)
C8—C15—C16—C17	-178.7 (2)	C14—C9—S1—N1	90.3 (2)
C15—C16—C17—C22	-149.4 (2)	C10—C9—S1—N1	-91.5 (2)
C15—C16—C17—C18	31.1 (4)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O2	0.93	2.37	2.949 (5)	120
C13—H13 $\cdots$ O1 <sup>i</sup>	0.93	2.73	3.420 (3)	132
C14—H14 $\cdots$ O2 <sup>ii</sup>	0.93	2.77	3.547 (4)	142
C19—H19 $\cdots$ Br1 <sup>iii</sup>	0.93	2.94	3.805 (3)	155
C5—H5 $\cdots$ Cg(C9—C14) <sup>iv</sup>	0.93	2.96	3.806 (4)	153
C23—H23A $\cdots$ Cg(C1—C6) <sup>iv</sup>	0.96	3.21	3.999 (3)	110
C23—H23B $\cdots$ Cg(N1/C1/C6—C8) <sup>v</sup>	0.96	3.12	3.561 (3)	149

Symmetry codes: (i)  $x, y-1, z$ ; (ii)  $-x+1/2, y-1/2, -z+1/2$ ; (iii)  $x, y+1, z$ ; (iv)  $-x+1, -y+1, -z+1$ ; (v)  $-x+1, -y+2, -z+1$ .