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Crystal structure and Hirshfeld analysis of 2-(5-bromothiophen-2-yl)acetonitrile

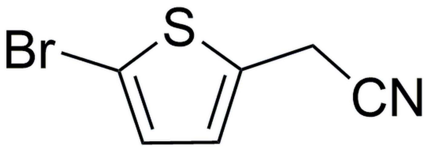
Ted M. Pappenfus,[a] Tiana L. Wood,[a] Joseph L. Morey,[a] Wyatt D. Wilcox[a] and Daron E. Janzen[b]*

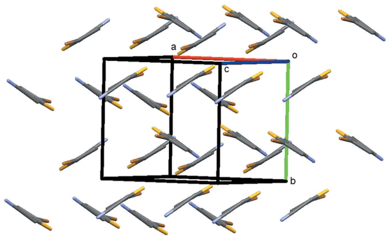
[a]Division of Science and Mathematics, University of Minnesota, Morris, MN 56267, USA, and [b]Dept. of Chemistry and Biochemistry, St. Catherine University, 20204 Randolph Avenue, St. Paul, MN 55105, USA. *Correspondence e-mail: dejanzen@stkate.edu

The title compound, C_6H_4BrNS, crystallizes in the space group $P2_1/n$ with one complete molecule in the asymmetric unit. The non-H atoms are nearly planar (r.m.s for non-H atoms = 0.071 Å), with the nitrile group oriented antiperiplanar with respect to the thiophene S atom. Intermolecular Type I centrosymmetric Br⋯Br halogen interactions are present at a distance of 3.582 (1) Å and with a C—Br⋯Br angle of 140.7 (1)°. Additional weaker C—H⋯N, C—H⋯S, and S⋯π interactions are also present. A Hirshfeld analysis indicates Br⋯Br interactions comprise only 1.9% of all the interatomic contacts.

1. Chemical context

Cyano-substituted molecules have found widespread use as functional materials for a variety of applications in organic electronics (Kim & Lim, 2014). For example, the title compound, 2-(5-bromothiophen-2-yl)acetonitrile, has been incorporated into materials for use in organic semiconductors (Park *et al.*, 2016), sensors (Ding *et al.*, 2015), dye-sensitized solar cells (Li *et al.*, 2016), and organic solar cells (Kwon *et al.*, 2015). Although the chemical literature has previously identified the title compound, **1**, as a liquid (Cho *et al.*, 2004; Chung *et al.*, 2009; Lu *et al.*, 2014; Wan *et al.*, 2009; Zou *et al.*, 2009), we have found that with proper purification, this molecule crystallizes under ambient conditions.





2. Structural commentary

The molecular structure of **1** is illustrated in Fig. 1. The asymmetric unit is composed of one complete molecule of **1**. The C1—C2, C2—C3, and C3—C4 bond lengths are consistent with some conjugation in the thienyl π-system (Table 1). While both the C4—C5 and C5—C6 bond lengths are consistent with single C—C bonds, the C5—C6 bond length is shorter, likely as a result of the *sp* hybridization at C6. Although conjugation across the molecule is not evident from the pattern of bond lengths, the structure is remarkably planar with an r.m.s. deviation from planarity of 0.071 Å for all non-hydrogen atoms.

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Table 1
Selected bond lengths (Å).

C1—C2	1.343 (6)	C4—C5	1.523 (7)
C2—C3	1.436 (6)	C5—C6	1.468 (7)
C3—C4	1.344 (7)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots$S1^{i}	0.95	2.93	3.844 (5)	162
C5—H5$B\cdots$N1^{ii}	0.99	2.66	3.425 (7)	134

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$.

3. Supramolecular Features

The structure packs with centrosymmetric π–π dimers, though the distance between least-squares planes formed by non-H atoms of the molecules is beyond the sum of the van der Waals radii at 3.637 Å. Molecules pack in a herringbone pattern with a dihedral angle of 65.2° between the least-squares planes formed by molecules related by the 2_1 screw axis (Fig. 2). The structure has several unique types of intermolecular features. Each molecule participates in centrosymmetric halogen-bonding dimers of Type I (Desiraju & Parthasarathy, 1989) with Br$\cdots$Br contacts at 3.582 (1) Å and a C1—Br1$\cdots$Br1 angle of 140.7 (1)° (Fig. 3). Each molecule also engages in two weaker C—H$\cdots$N interactions, one as an sp^3-hybridized C5—H5*B* donor and the other as an acceptor (N1) of this type of interaction (Table 2, Fig. 4). It is noteworthy that the two methylene hydrogen atoms are acidic on account of the electron-withdrawing nature of the cyano group and hence their participation in the formation of C—H$\cdots$N hydrogen bonds is significant. Additionally, atom S1 contributes to two unique intermolecular interactions. S1 acts as acceptor for an interaction with C3—H3 as the donor. These S$\cdots$H interactions are organized in a $C_1^1(4)$ graph-set motif parallel to [101]. An edge-to-face S1$\cdots\pi$(C1—C2 midpoint) interaction is also present at a distance of 3.391 Å (sum of van der Waals radii = 3.50 Å). These S$\cdots\pi$ close contacts are organized in chains parallel to [010].

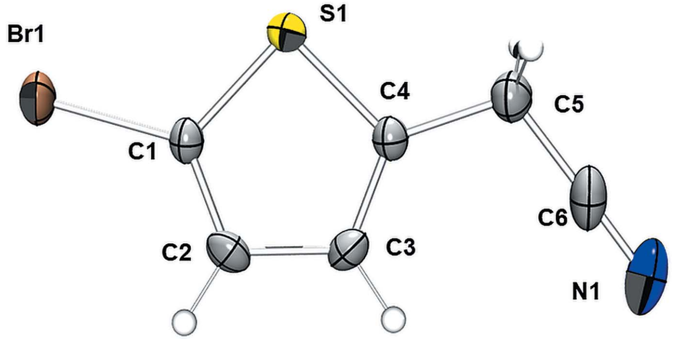

Figure 1
A displacement ellipsoid plot (50% probability ellipsoids for non-H atoms) of the asymmetric unit of **1**.

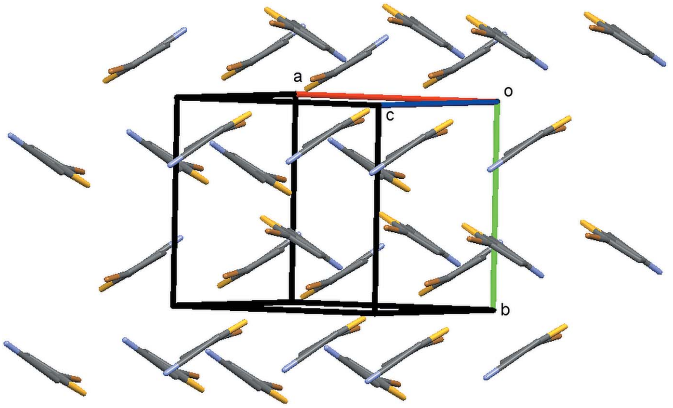

Figure 2
Packing diagram of **1** showing the herringbone packing pattern.

4. Hirshfeld surface analysis

Intermolecular interactions were studied further through analysis of the Hirshfeld surface, generated using *CrystalExplorer* (McKinnon *et al.* 2007; Spackman & Jayatilaka, 2009). Fig. 5 shows two orientations of the Hirshfeld surface mapped over $d_{\rm norm}$. The red areas of the surface indicate negative $d_{\rm norm}$ values corresponding to contacts closer than the sum of van der Waals radii and highlight the relevant intermolecular interactions discussed. The relative surface-area contributions from the particular interatomic contacts

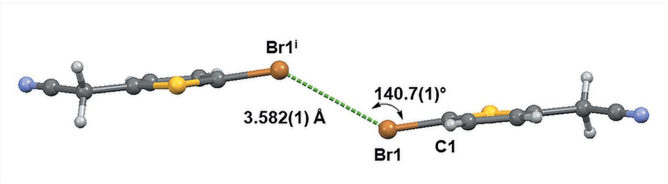

Figure 3
Intermolecular halogen interaction of **1**. Symmetry code: (i) $2-x, -y, 1-z$.

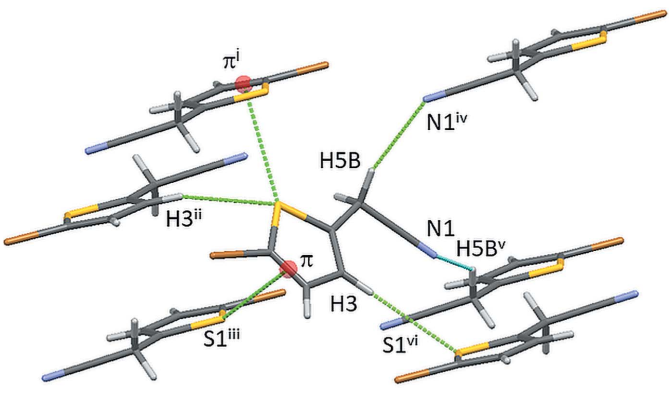

Figure 4
Intermolecular interactions of **1**. Br$\cdots$Br interactions omitted for clarity. π indicates the C1—C2 midpoint. Symmetry codes: (i) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (ii) $-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (iv) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{5}{2}-z$; (v) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{5}{2}-z$; (vi) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface.

Contact	%
N···H/H···N	21.8
S···H/H···S	10.3
S···C/C···S	6.9
C···C	4.1
Br···Br	1.9

described for **1** to the total Hirshfeld surfaces are summarized in Table 3. While N···H contacts comprise the largest percentage of contacts to the Hirshfeld surface described, the angular and distance components involved in the C—H···N hydrogen-bonding interactions do not suggest that these interactions dominate the packing. The Br···Br contacts comprise the smallest percentage of interatomic contacts described, however these Br···Br atom contacts [3.582 (1) Å] are the shortest of all the contacts described, relative to the van der Waals radii sums (−0.118 Å). The observation that C···C contacts comprise only a small percentage of the interatomic contacts is consistent with minor π–π stacking contributions and the observed stacking distance beyond the sum of the van der Waals radii.

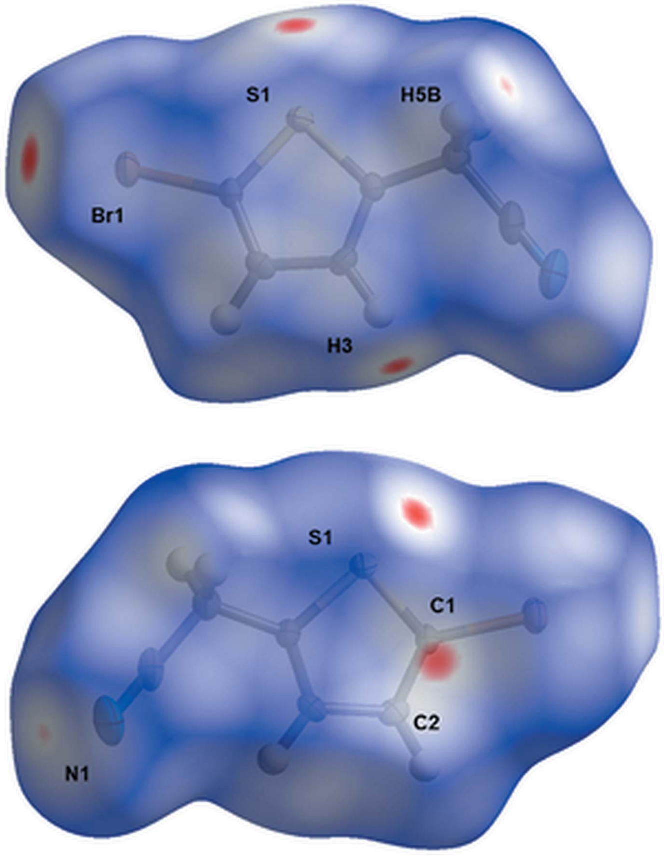

Figure 5
Hirshfeld surface of **1** mapped over $d_{\rm norm}$, shown in two orientations in the range −0.0639 to 0.93667 a.u. Red areas highlight intermolecular contacts shorter than the sum of the van der Waals radii.

5. Database Survey

A search of the current version of the Cambridge Structural Database (Version 5.39, updated November 2017; Groom *et al.*, 2016) yields a number of related structures with a 5-bromothiophene fragment but only two non-salt structures with exclusively one small substituent in the 2-position. The structure of 2-acetyl-5-bromothiophene (ACBTHO; Streurman & Schenk, 1970) is planar like **1**, but the acetyl group is syn-periplanar relative to the sulfur of thiophene, and Br···O=C interactions are present in the absence of Br···Br interactions. The structure of a co-crystal of 5-bromothiophene-2-carboxylic acid with 5-fluorouracil (CAWCAP; Mohana *et al.*, 2017) is also similar, with no Br···Br interactions but the presence of Br···O=C interactions. No other structures of any substituted 2-thiopheneacetonitrile have been reported.

The Type I Br···Br halogen-interaction pattern of **1** is very similar to three other structures reported with only one bromine donor in the 5-position and no substitution in the 3- or 4-positions of the thiophene group. The structures of 2-bromo-5-[4-(4-nitrophenyl)buta-1,3-dien-1-yl]thiophene (MUJTUH; Kanibolotsky *et al.*, 2009), (2*E*)-1-(5-bromo-2-thienyl)-3-(4-ethylphenyl)prop-2-en-1-one (PUSKUL; Naik *et al.*, 2015), and (2*RS*,4*SR*)-2-exo-(5-bromo-2-thienyl)-7-chloro-2,3,4,5-tetrahydro-1*H*-1,4-epoxy-1-benzazepine (YUCTIA; Blanco *et al.*, 2009) have short intermolecular Br···Br contacts with distances of 3.4619 (4), 3.4917 (5), and 3.5234 (7) Å, respectively, and centrosymmetric interactions with C—Br···Br angles of 145.12 (9), 151.37 (8), and 143.8 (1)°, respectively.

6. Synthesis and Crystallization

The title compound, 2-(5-bromothiophen-2-yl)acetonitrile, was prepared according to the literature procedure (Lu *et al.*, 2014). Additional purification was performed by vacuum distillation (b.p. 334 K @ 0.07 mm Hg), which provided a colorless liquid that crystallized over several days to afford colorless crystals (m.p. 302–305 K) suitable for X-ray diffraction. EI–MS m/z (relative intensity) 202.88 (29.9), 200.89 (29.7), 123.02 (8.6), 122.01 (100.0), 95.03 (11.1).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. H atoms were placed in calculated positions and refined in the riding-model approximation with distances of C—H = 0.95 and 0.99 Å for the thiophene and methylene groups, respectively, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

A single low-angle reflection was rejected from these high-quality data sets due to the arrangement of the instrument with a conservatively sized beam stop and a fixed-position detector. The large number of reflections in the data sets (and the Fourier-transform relationship of intensities to atoms) ensures that no particular bias was thereby introduced.

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Table 4
Experimental details.

Crystal data	
Chemical formula	C_6H_4BrNS
M_r	202.07
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	9.775 (4), 7.278 (3), 10.698 (4)
β (°)	110.933 (8)
V (Å^3)	710.8 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	6.00
Crystal size (mm)	0.51 × 0.44 × 0.22
Data collection	
Diffractometer	Rigaku XtaLAB mini
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
$T_{\min}$, $T_{\max}$	0.141, 0.267
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	6585, 1444, 1198
$R_{\rm int}$	0.048
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.117, 1.07
No. of reflections	1444
No. of parameters	82
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.55, −0.82

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2011), *SIR2004* (Burla *et al.*, 2005), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *publCIF* (Westrip, 2010) and *CrystalStructure* (Rigaku, 2014).

supporting information

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Crystal structure and Hirshfeld analysis of 2-(5-bromothiophen-2-yl)acetonitrile

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Computing details

Data collection: *CrystalClear-SM Expert* (Rigaku, 2011); cell refinement: *CrystalClear-SM Expert* (Rigaku, 2011); data reduction: *CrystalClear-SM Expert* (Rigaku, 2011); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2014).

2-(5-Bromothiophen-2-yl)acetonitrile

Crystal data

C_6H_4BrNS
$M_r = 202.07$
Monoclinic, $P2_1/n$
$a = 9.775$ (4) Å
$b = 7.278$ (3) Å
$c = 10.698$ (4) Å
$\beta = 110.933$ (8)°
$V = 710.8$ (5) Å^3
$Z = 4$

$F(000) = 392.00$
$D_x = 1.888$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 5750 reflections
$\theta = 3.5$–26.5°
$\mu = 6.00$ mm^{-1}
$T = 173$ K
Prism, colorless
0.51 × 0.44 × 0.22 mm

Data collection

Rigaku XtaLAB mini diffractometer
Detector resolution: 6.849 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
$T_{min} = 0.141$, $T_{max} = 0.267$
6585 measured reflections

1444 independent reflections
1198 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int} = 0.048$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.5°$
$h = -12 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.117$
$S = 1.07$
1444 reflections
82 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
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-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.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Br1	0.90954 (6)	0.12818 (8)	0.59072 (5)	0.0348 (2)
S1	0.76060 (13)	0.07396 (16)	0.79952 (11)	0.0242 (3)
N1	0.8679 (6)	0.3162 (8)	1.2745 (5)	0.0610 (16)
C1	0.9070 (5)	0.1545 (6)	0.7644 (4)	0.0218 (10)
C2	1.0043 (5)	0.2468 (6)	0.8663 (4)	0.0258 (11)
H2	1.0914	0.3016	0.8634	0.031*
C3	0.9592 (5)	0.2517 (6)	0.9801 (5)	0.0261 (11)
H3	1.0143	0.3093	1.0624	0.031*
C4	0.8308 (5)	0.1662 (6)	0.9581 (4)	0.0220 (10)
C5	0.7453 (6)	0.1396 (6)	1.0510 (5)	0.0314 (12)
H5A	0.6437	0.1841	1.0063	0.038*
H5B	0.7410	0.0071	1.0701	0.038*
C6	0.8137 (6)	0.2395 (7)	1.1774 (5)	0.0382 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0342 (4)	0.0494 (4)	0.0253 (3)	−0.0001 (2)	0.0160 (3)	−0.0028 (2)
S1	0.0219 (7)	0.0271 (6)	0.0233 (6)	−0.0037 (5)	0.0077 (5)	−0.0011 (5)
N1	0.079 (5)	0.077 (4)	0.038 (3)	0.001 (3)	0.034 (3)	−0.012 (3)
C1	0.023 (3)	0.025 (2)	0.019 (2)	0.0048 (19)	0.0088 (19)	0.0027 (17)
C2	0.016 (3)	0.029 (3)	0.032 (3)	0.0024 (19)	0.008 (2)	0.0032 (19)
C3	0.026 (3)	0.027 (3)	0.021 (2)	0.001 (2)	0.005 (2)	−0.0052 (18)
C4	0.023 (3)	0.024 (2)	0.021 (2)	0.0026 (19)	0.009 (2)	0.0022 (18)
C5	0.034 (3)	0.036 (3)	0.027 (3)	0.000 (2)	0.013 (2)	0.002 (2)
C6	0.044 (4)	0.049 (4)	0.028 (3)	0.011 (3)	0.021 (3)	0.006 (2)

Geometric parameters (Å, º)

Br1—C1	1.877 (4)	C3—C4	1.344 (7)
S1—C1	1.708 (5)	C3—H3	0.9500
S1—C4	1.723 (4)	C4—C5	1.523 (7)
N1—C6	1.131 (7)	C5—C6	1.468 (7)
C1—C2	1.343 (6)	C5—H5A	0.9900
C2—C3	1.436 (6)	C5—H5B	0.9900
C2—H2	0.9500		

C1—S1—C4	90.7 (2)	C3—C4—C5	129.8 (4)
C2—C1—S1	113.5 (4)	C3—C4—S1	111.8 (3)
C2—C1—Br1	126.8 (4)	C5—C4—S1	118.4 (3)
S1—C1—Br1	119.4 (3)	C6—C5—C4	111.2 (4)
C1—C2—C3	110.9 (4)	C6—C5—H5A	109.4
C1—C2—H2	124.5	C4—C5—H5A	109.4
C3—C2—H2	124.5	C6—C5—H5B	109.4
C4—C3—C2	113.0 (4)	C4—C5—H5B	109.4
C4—C3—H3	123.5	H5A—C5—H5B	108.0
C2—C3—H3	123.5	N1—C6—C5	179.2 (6)

C4—S1—C1—C2	−0.1 (4)	C2—C3—C4—S1	0.8 (5)
C4—S1—C1—Br1	−174.5 (3)	C1—S1—C4—C3	−0.4 (4)
S1—C1—C2—C3	0.6 (5)	C1—S1—C4—C5	−179.6 (4)
Br1—C1—C2—C3	174.5 (3)	C3—C4—C5—C6	5.7 (7)
C1—C2—C3—C4	−0.9 (6)	S1—C4—C5—C6	−175.2 (3)
C2—C3—C4—C5	179.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···S1^{i}	0.95	2.93	3.844 (5)	162
C5—H5*B*···N1^{ii}	0.99	2.66	3.425 (7)	134

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+5/2.