

# Crystal structure of 1-(1,3-benzothiazol-2-yl)-3-(4-bromobenzoyl)thiourea

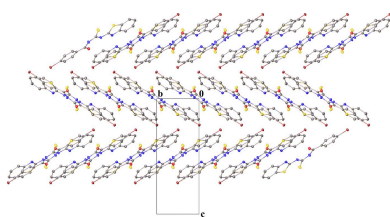
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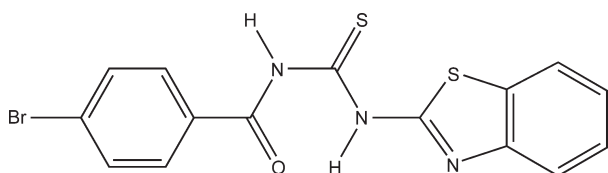
The chemical reaction of 4-bromobenzoylchloride and 2-aminothiazole in the presence of potassium thiocyanate yielded a white solid formulated as  $C_{15}H_{10}BrN_3OS_2$ , which consists of 4-bromobenzamido and 2-benzothiazolyl moieties connected by a thiourea group. The 4-bromobenzamido and 2-benzothiazolyl moieties are in a *trans* conformation (sometimes also called *s-trans* due to the single bond) with respect to the N–C bond. The dihedral angle between the mean planes of the 4-bromophenyl and the 2-benzothiazolyl units is  $10.45(11)^\circ$ . The thiourea moiety,  $-C-NH-C(=S)-NH-$  fragment forms a dihedral angle of  $8.64(12)^\circ$  with the 4-bromophenyl ring and is almost coplanar with the 2-benzothiazolyl moiety, with a dihedral angle of  $1.94(11)^\circ$ . The molecular structure is stabilized by intramolecular N–H $\cdots$ O hydrogen bonds, resulting in the formation of an *S*(6) ring. In the crystal, pairs of adjacent molecules interact *via* intermolecular hydrogen bonds of type C–H $\cdots$ N, C–H $\cdots$ S and N–H $\cdots$ S, resulting in molecular layers parallel to the *ac* plane.

## 1. Chemical context

Benzimidazole is a heterocycle widely used in the development of therapeutic molecules. Several drugs are being developed around the world and researchers continue to be interested in benzimidazole derivatives and their applications (Awadh, 2023; Dhanamjayulu *et al.*, 2023; Mavvaji & Akkoc, 2024; Bandaru *et al.*, 2023). Benzimidazole derivatives with anticancer (Abbade *et al.*, 2024), antihistamine (Wang *et al.*, 2012), antiviral (Mahurkar *et al.*, 2023), antimicrobial (Bhoi *et al.*, 2023), antituberculous (Kalalbandi *et al.*, 2014), anti-diabetic (Saeedian Moghadam *et al.*, 2023), anti-inflammatory (Nagesh *et al.*, 2022), antioxidant (Patagar *et al.*, 2023) and antifungal (Çevik *et al.*, 2022) properties have been reported in the literature. Thiourea has interesting chemical properties, which have made it possible to develop several applications (Abdelgawad *et al.*, 2023; Fiaz *et al.*, 2024; Huang *et al.*, 2023; Eshkil *et al.*, 2017). Its high reactivity has made it possible to synthesize a very large number of derivatives with analgesic (Lee *et al.*, 2002), anticancer (Pingaew *et al.*, 2022), antimicrobial (Madasani *et al.*, 2023), and antidiabetic (Faidallah *et al.*, 2011) properties. The combination of thiourea and benzimidazole made it possible to generate new molecules with properties better than those of derivatives of the two uncombined molecules (Ganesh *et al.*, 2015; Harrouche *et al.*, 2016; Shang *et al.*, 2023). Molecules derived from benzimidazole-thiourea presenting potent antiproliferative activity, compared to reference drugs, have been synthesized (Ullah *et al.*, 2022; Siddiq *et al.*, 2021). It is in this context that thiourea



derivatives are the subject of particular interest for researchers seeking to develop molecules containing one or more metal ions to improve the properties of these compounds (Muhammed *et al.*, 2024; Albrecht *et al.*, 2024; Nair *et al.*, 2022; Masaryk *et al.*, 2021). Complexes exhibiting biological properties are reported in the literature (Zhao *et al.*, 2024; Swaminathan *et al.*, 2024; Muhammed *et al.*, 2024; Albrecht *et al.*, 2024). For several years, our research group has been developing compounds containing the thiourea moiety (Faye, Gaye *et al.*, 2022; Faye, Mbow *et al.*, 2022; Thiam *et al.*, 2008; Samb *et al.*, 2019). In this work, we report the synthesis and characterization of a molecule containing both thiourea and benzimidazole moieties.



## 2. Structural commentary

The X-ray structure determination revealed that the title compound crystallizes in the monoclinic space group  $P2_1/n$  with one molecule in the asymmetric unit. The molecular geometry is illustrated in Fig. 1. The S1—C1 [1.745 (2) Å] and the S1—C7 [1.751 (2) Å] distances indicate that these correspond to single bonds. The S2—C8 [1.663 (2) Å] and the O1—C9 [1.220 (2) Å] and N1—C7 [1.291 (3) Å] distances indicate that these correspond to double bonds and are comparable to those observed for 1,2-bis(*N'*-benzoylthioureido)benzene [1.6574 (18) Å for C—S, 1.219 (2) Å and 1.224 (3) Å for C—O; Thiam *et al.*, 2008]. The N1—C7 [1.291 (3) Å] distance indicates double-bond character, similar to the corresponding bond length in (*Z*)-2-[(*E*)-2-(1-benzothiofene-3-ylmethylidene)hydrazin-1-ylidene]-1,2-diphenylethane [1.281 (3) Å; Pekdemir *et al.*, 2012]. The N1—C6 [1.392 (3) Å], N2—C7 [1.390 (3) Å], N3—C8 [1.386 (3) Å] and N3—C9 [1.383 (3) Å] distances are in the normal range observed for a single C—N bond (Samb *et al.*, 2019; Chen *et al.*, 2001). The bond angles around N2, N3 and C8 fall in the range 115.40 (17)–128.81 (17)° and are comparable to the ideal value of 120° observed for  $sp^2$  hybridization. The phenyl ring and the benzothiazole ring are essentially planar with

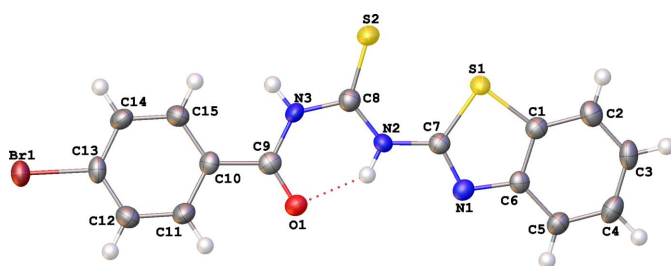


Figure 1

A view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 30% probability level.

Table 1

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>
N3—H3···S2 <sup>i</sup>	0.88	2.96	3.6102 (19)	132
N2—H2···O1	0.88	1.90	2.633 (2)	139
C14—H14···S2 <sup>ii</sup>	0.95	2.95	3.779 (2)	146
C2—H2A···S1 <sup>iii</sup>	0.95	3.00	3.908 (2)	161
C5—H5···N1 <sup>iv</sup>	0.95	2.68	3.604 (3)	165

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

r.m.s deviations of 0.0081 and 0.0070 Å, respectively. The thiourea fragment (S2/N3/N2/C8/C9) is planar with a maximum deviation from its mean plane of 0.0519 (1) Å for N3. The 4-bromophenyl ring and the 2-benzothiazolyl groups are twisted relative to each other and form a dihedral angle of 10.45 (11)°. The two rings make dihedral angles of 8.64 (12) and 1.94 (11)°, respectively, with the thiourea fragment. The 4-bromobenzoyl group is *trans* with respect to the thiono S atom across the N3—C8 bond. The 2-benzothiazolyl ring adopts a *cis* conformation with respect to the thiono S atom across the N2—C8 bond. The molecule exhibits an intramolecular N—H···O hydrogen bond (Table 1) between the carbonyl oxygen atom and the thioamide hydrogen atom, which forms an *S*(6) ring. This phenomenon is regularly noted in the case of carbonylurea and benzoyl thiourea (Sow *et al.*, 2009; Woei Hung & Kassim, 2010) derivatives.

## 3. Supramolecular features

In the crystal, the molecules are linked into chains that are connected by intermolecular hydrogen bonds of type C—H···N, C—H···S, and N—H···S (Table 1), forming molecular layers running parallel to the *ac* plane. Intermolecular N—H···S and C—H···N hydrogen bonds further link the molecules, forming a zigzag chain through  $R_2^2(8)$  rings. The intermolecular C—H···S hydrogen bond consolidates the structure, forming rings of type  $R_2^1(8)$  (Figs. 2 and 3).

## 4. Database survey

A search of the Cambridge Structural Database (CSD version 5.44, updates of September 2023; Groom *et al.*, 2016) with the

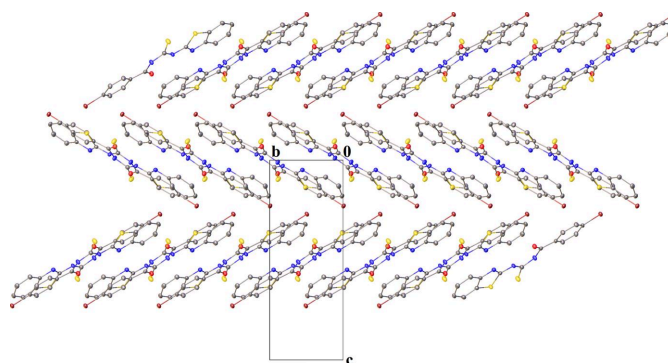
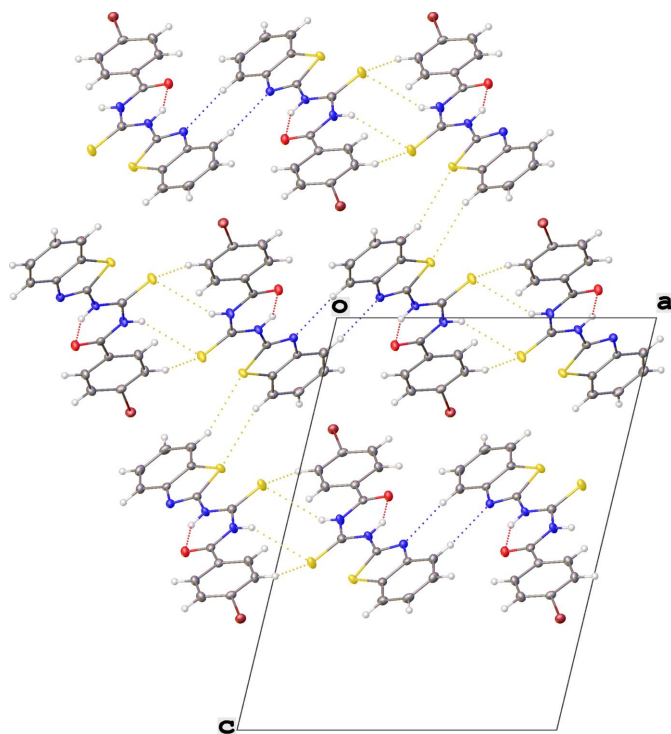


Figure 2

Partial packing view along the *a* axis, H atoms are omitted for clarity.



**Figure 3**  
Partial packing view down the  $b$  axis showing the formation of  $R_2^2(8)$  graph-set motifs. Hydrogen bonds are drawn as dashed lines.

search fragment benzothiazole thiourea yielded seventeen hits. For some hits, the bromine atom is replaced by a chlorine atom (BUDZIK; Yusof *et al.*, 2009) or nitro group (HUWIM; Cui *et al.*, 2009). Other results give the same chemical formula and structure but have the bromine atom in the *ortho* or *meta* position on the benzene ring [IVEWEO (Zeng *et al.*, 2017) and SURGOE (Odame *et al.*, 2020)]. Coordination complexes based on transition metals such as rhenium (INOXUG; Schoultz *et al.*, 2016), ruthenium (NODLUQ; Shadap *et al.*, 2019) and rhodium (NODMAX; Shadap *et al.*, 2019) have organic ligands that are analogues of the reported molecule.

## 5. Synthesis and crystallization

The title compound was synthesized following the procedure reported by Odame *et al.* (2020) with slight modification. The thiourea derivative was obtained by the reaction of potassium thiocyanate (1.9388 g, 20 mmol) with 4-bromobenzoyl chloride (4.3892 g, 20 mmol) in 25 mL of acetone and heating under reflux for 2 h to yield the 4-bromobenzoyl isothiocyanate. To the above solution was added a solution of 2-aminobenzothiazole (3 g, 20 mmol) in 25 mL of acetone. The resulting mixture was heated overnight. The solvent was removed by evaporation and the crude product was recrystallized in methanol. Yield 77%, m.p. 504 K. Analysis calculated for  $C_{15}H_{10}BrN_3OS_2$ : C, 45.92; H, 2.57; N, 10.71; S, 16.35. Found: C, 45.90; H, 2.55; N, 10.69; S, 16.32. FTIR: ( $\nu$ ,  $\text{cm}^{-1}$ ): 3075 (N–H), 3015 (N–H), 1675 (C=O), 1563 (C=C), 1546 (C=C), 1451 (C–N), 1439 (C–N).

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}BrN_3OS_2$
$M_r$	392.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
$a, b, c$ (Å)	13.5009 (5), 6.4130 (2), 17.9147 (7)
$\beta$ (°)	103.606 (4)
$V$ (Å <sup>3</sup> )	1507.54 (10)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	3.01
Crystal size (mm)	0.10 × 0.06 × 0.06
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian ( <i>CrysAlis PRO</i> ; Rigaku OD, 2022)
$T_{\min}, T_{\max}$	0.804, 0.986
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	18792, 3074, 2581
$R_{\text{int}}$	0.041
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.024, 0.057, 1.03
No. of reflections	3074
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.35, −0.30

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were geometrically optimized (C–H = 0.95 Å, N–H = 0.88 Å) and refined as riding on their carriers with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ .

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## supporting information

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## Crystal structure of 1-(1,3-benzothiazol-2-yl)-3-(4-bromobenzoyl)thiourea

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### Computing details

#### 1-(1,3-Benzothiazol-2-yl)-3-(4-bromobenzoyl)thiourea

##### Crystal data

$C_{15}H_{10}BrN_3OS_2$

$M_r = 392.29$

Monoclinic,  $P2_1/n$

$a = 13.5009$  (5) Å

$b = 6.4130$  (2) Å

$c = 17.9147$  (7) Å

$\beta = 103.606$  (4)°

$V = 1507.54$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 784$

$D_x = 1.728$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9123 reflections

$\theta = 3.1$ – $33.9$ °

$\mu = 3.01$  mm<sup>-1</sup>

$T = 100$  K

Block, light colourless

$0.10 \times 0.06 \times 0.06$  mm

##### Data collection

XtaLAB Synergy, Dualflex, HyPix  
diffractometer

Detector resolution: 10.0000 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: gaussian  
(CrysAlisPro; Rigaku OD, 2022)

$T_{\min} = 0.804$ ,  $T_{\max} = 0.986$

18792 measured reflections

3074 independent reflections

2581 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 26.4$ °,  $\theta_{\min} = 3.1$ °

$h = -16$ → $16$

$k = -8$ → $8$

$l = -22$ → $21$

##### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.057$

$S = 1.03$

3074 reflections

199 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0191P)^2 + 1.3729P]$

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

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

$\Delta\rho_{\max} = 0.35$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.30$  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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.07298 (2)	−0.50717 (3)	0.27034 (2)	0.01865 (7)
S1	0.24869 (4)	0.98772 (8)	0.63447 (3)	0.01659 (12)
S2	0.10718 (4)	0.61809 (8)	0.59446 (3)	0.02191 (13)
O1	0.29683 (11)	0.3918 (2)	0.43225 (8)	0.0182 (3)
N3	0.16341 (14)	0.3897 (3)	0.48987 (10)	0.0172 (4)
H3	0.106967	0.322341	0.490909	0.021*
N1	0.38000 (13)	0.9461 (3)	0.54899 (10)	0.0155 (4)
N2	0.26397 (13)	0.6774 (3)	0.52923 (10)	0.0148 (4)
H2	0.298111	0.627829	0.496902	0.018*
C10	0.18323 (16)	0.1035 (3)	0.40497 (12)	0.0145 (4)
C11	0.24401 (17)	0.0071 (3)	0.36228 (12)	0.0183 (4)
H11	0.307296	0.068130	0.359855	0.022*
C8	0.18301 (16)	0.5657 (3)	0.53592 (12)	0.0167 (4)
C9	0.22053 (16)	0.3057 (3)	0.44251 (12)	0.0152 (4)
C13	0.12063 (17)	−0.2631 (3)	0.32704 (12)	0.0162 (4)
C6	0.40504 (15)	1.1298 (3)	0.59049 (11)	0.0139 (4)
C4	0.49993 (17)	1.4411 (3)	0.62991 (13)	0.0208 (5)
H4	0.553913	1.533414	0.626970	0.025*
C12	0.21305 (17)	−0.1773 (3)	0.32321 (13)	0.0199 (5)
H12	0.254784	−0.243387	0.294303	0.024*
C14	0.05956 (16)	−0.1731 (3)	0.37025 (13)	0.0178 (4)
H14	−0.003263	−0.235813	0.372947	0.021*
C3	0.43652 (17)	1.4872 (3)	0.67971 (13)	0.0200 (5)
H3A	0.448160	1.611081	0.709576	0.024*
C2	0.35797 (17)	1.3570 (3)	0.68620 (12)	0.0196 (5)
H2A	0.315825	1.387679	0.720416	0.023*
C1	0.34260 (16)	1.1782 (3)	0.64059 (12)	0.0158 (4)
C7	0.30166 (16)	0.8612 (3)	0.56641 (12)	0.0144 (4)
C15	0.09165 (17)	0.0100 (3)	0.40956 (13)	0.0185 (4)
H15	0.050806	0.072576	0.439944	0.022*
C5	0.48474 (16)	1.2633 (3)	0.58523 (12)	0.0179 (4)
H5	0.527660	1.232504	0.551582	0.021*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.02144 (12)	0.01489 (11)	0.01875 (12)	−0.00221 (8)	0.00297 (8)	−0.00376 (8)
S1	0.0190 (3)	0.0164 (2)	0.0168 (3)	−0.0037 (2)	0.0090 (2)	−0.0033 (2)
S2	0.0203 (3)	0.0227 (3)	0.0263 (3)	−0.0068 (2)	0.0127 (2)	−0.0073 (2)
O1	0.0163 (8)	0.0172 (7)	0.0223 (8)	−0.0017 (6)	0.0071 (6)	−0.0016 (6)
N3	0.0164 (9)	0.0160 (9)	0.0212 (10)	−0.0064 (7)	0.0087 (8)	−0.0048 (7)
N1	0.0149 (9)	0.0163 (8)	0.0154 (9)	−0.0014 (7)	0.0036 (7)	0.0004 (7)
N2	0.0159 (9)	0.0147 (8)	0.0158 (9)	−0.0021 (7)	0.0074 (7)	−0.0038 (7)
C10	0.0162 (11)	0.0115 (10)	0.0150 (11)	−0.0002 (8)	0.0020 (9)	0.0018 (8)
C11	0.0174 (11)	0.0187 (11)	0.0199 (11)	−0.0035 (9)	0.0070 (9)	−0.0006 (9)

C8	0.0173 (11)	0.0165 (10)	0.0160 (11)	-0.0008 (8)	0.0035 (9)	0.0001 (8)
C9	0.0150 (11)	0.0161 (10)	0.0136 (11)	0.0012 (8)	0.0014 (9)	0.0034 (8)
C13	0.0204 (12)	0.0114 (9)	0.0147 (11)	-0.0012 (8)	-0.0002 (9)	-0.0008 (8)
C6	0.0139 (11)	0.0141 (10)	0.0123 (10)	0.0006 (8)	0.0004 (8)	0.0003 (8)
C4	0.0182 (12)	0.0189 (11)	0.0231 (12)	-0.0050 (9)	0.0004 (9)	0.0008 (8)
C12	0.0209 (12)	0.0195 (11)	0.0210 (12)	0.0005 (9)	0.0086 (10)	-0.0024 (9)
C14	0.0147 (11)	0.0166 (10)	0.0233 (12)	-0.0020 (8)	0.0066 (9)	0.0003 (8)
C3	0.0231 (12)	0.0151 (10)	0.0185 (11)	-0.0018 (9)	-0.0016 (9)	-0.0037 (8)
C2	0.0219 (12)	0.0198 (11)	0.0161 (11)	0.0002 (9)	0.0026 (9)	-0.0021 (8)
C1	0.0158 (11)	0.0171 (10)	0.0142 (11)	-0.0009 (8)	0.0029 (9)	0.0011 (8)
C7	0.0155 (11)	0.0152 (10)	0.0124 (10)	-0.0002 (8)	0.0031 (8)	0.0013 (8)
C15	0.0187 (11)	0.0175 (10)	0.0210 (12)	-0.0002 (9)	0.0081 (9)	-0.0018 (9)
C5	0.0155 (11)	0.0184 (10)	0.0197 (11)	-0.0024 (8)	0.0037 (9)	-0.0008 (8)

*Geometric parameters (Å, °)*

Br1—C13	1.894 (2)	C11—C12	1.388 (3)
S1—C1	1.745 (2)	C13—C12	1.380 (3)
S1—C7	1.751 (2)	C13—C14	1.383 (3)
S2—C8	1.663 (2)	C6—C1	1.403 (3)
O1—C9	1.220 (2)	C6—C5	1.396 (3)
N3—H3	0.8800	C4—H4	0.9500
N3—C8	1.386 (3)	C4—C3	1.406 (3)
N3—C9	1.383 (3)	C4—C5	1.380 (3)
N1—C6	1.392 (3)	C12—H12	0.9500
N1—C7	1.291 (3)	C14—H14	0.9500
N2—H2	0.8800	C14—C15	1.386 (3)
N2—C8	1.335 (3)	C3—H3A	0.9500
N2—C7	1.390 (3)	C3—C2	1.376 (3)
C10—C11	1.391 (3)	C2—H2A	0.9500
C10—C9	1.492 (3)	C2—C1	1.395 (3)
C10—C15	1.394 (3)	C15—H15	0.9500
C11—H11	0.9500	C5—H5	0.9500
C1—S1—C7	87.61 (9)	C5—C4—H4	119.6
C8—N3—H3	115.6	C5—C4—C3	120.8 (2)
C9—N3—H3	115.6	C11—C12—H12	120.6
C9—N3—C8	128.78 (18)	C13—C12—C11	118.89 (19)
C7—N1—C6	109.74 (17)	C13—C12—H12	120.6
C8—N2—H2	115.6	C13—C14—H14	120.6
C8—N2—C7	128.81 (17)	C13—C14—C15	118.80 (19)
C7—N2—H2	115.6	C15—C14—H14	120.6
C11—C10—C9	116.96 (18)	C4—C3—H3A	119.3
C11—C10—C15	119.18 (19)	C2—C3—C4	121.5 (2)
C15—C10—C9	123.85 (18)	C2—C3—H3A	119.3
C10—C11—H11	119.7	C3—C2—H2A	121.3
C12—C11—C10	120.6 (2)	C3—C2—C1	117.4 (2)
C12—C11—H11	119.7	C1—C2—H2A	121.3

N3—C8—S2	118.68 (15)	C6—C1—S1	110.00 (15)
N2—C8—S2	125.92 (16)	C2—C1—S1	128.16 (16)
N2—C8—N3	115.40 (17)	C2—C1—C6	121.83 (19)
O1—C9—N3	121.88 (19)	N1—C7—S1	117.69 (15)
O1—C9—C10	122.19 (18)	N1—C7—N2	118.04 (18)
N3—C9—C10	115.92 (18)	N2—C7—S1	124.26 (15)
C12—C13—Br1	119.98 (16)	C10—C15—H15	119.7
C12—C13—C14	121.79 (19)	C14—C15—C10	120.69 (19)
C14—C13—Br1	118.22 (16)	C14—C15—H15	119.7
N1—C6—C1	114.95 (18)	C6—C5—H5	120.7
N1—C6—C5	125.29 (18)	C4—C5—C6	118.65 (19)
C5—C6—C1	119.76 (18)	C4—C5—H5	120.7
C3—C4—H4	119.6		
Br1—C13—C12—C11	176.90 (16)	C12—C13—C14—C15	1.1 (3)
Br1—C13—C14—C15	-177.46 (16)	C14—C13—C12—C11	-1.7 (3)
N1—C6—C1—S1	-0.6 (2)	C3—C4—C5—C6	0.0 (3)
N1—C6—C1—C2	179.95 (19)	C3—C2—C1—S1	-178.55 (17)
N1—C6—C5—C4	179.7 (2)	C3—C2—C1—C6	0.8 (3)
C10—C11—C12—C13	0.4 (3)	C1—S1—C7—N1	0.05 (18)
C11—C10—C9—O1	5.2 (3)	C1—S1—C7—N2	-178.98 (19)
C11—C10—C9—N3	-174.74 (18)	C1—C6—C5—C4	0.0 (3)
C11—C10—C15—C14	-2.0 (3)	C7—S1—C1—C6	0.32 (16)
C8—N3—C9—O1	-4.8 (3)	C7—S1—C1—C2	179.7 (2)
C8—N3—C9—C10	175.1 (2)	C7—N1—C6—C1	0.7 (3)
C8—N2—C7—S1	1.2 (3)	C7—N1—C6—C5	-179.1 (2)
C8—N2—C7—N1	-177.8 (2)	C7—N2—C8—S2	-2.1 (3)
C9—N3—C8—S2	-173.64 (17)	C7—N2—C8—N3	178.90 (19)
C9—N3—C8—N2	5.5 (3)	C15—C10—C11—C12	1.5 (3)
C9—C10—C11—C12	-177.60 (19)	C15—C10—C9—O1	-173.8 (2)
C9—C10—C15—C14	177.0 (2)	C15—C10—C9—N3	6.2 (3)
C13—C14—C15—C10	0.7 (3)	C5—C6—C1—S1	179.10 (16)
C6—N1—C7—S1	-0.4 (2)	C5—C6—C1—C2	-0.3 (3)
C6—N1—C7—N2	178.69 (17)	C5—C4—C3—C2	0.5 (3)
C4—C3—C2—C1	-0.8 (3)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3 $\cdots$ S2 <sup>i</sup>	0.88	2.96	3.6102 (19)	132
N2—H2 $\cdots$ O1	0.88	1.90	2.633 (2)	139
C14—H14 $\cdots$ S2 <sup>ii</sup>	0.95	2.95	3.779 (2)	146
C2—H2A $\cdots$ S1 <sup>iii</sup>	0.95	3.00	3.908 (2)	161
C5—H5 $\cdots$ N1 <sup>iv</sup>	0.95	2.68	3.604 (3)	165

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