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## Structure Reports

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# 1,5-Bis[1-(4-bromophenyl)ethylidene]-thiocarbonohydrazide

Zhiqing Gao

Dongchang College, Liaocheng University, Liaocheng 250059, People's Republic of China

Correspondence e-mail: gaozq08@163.com

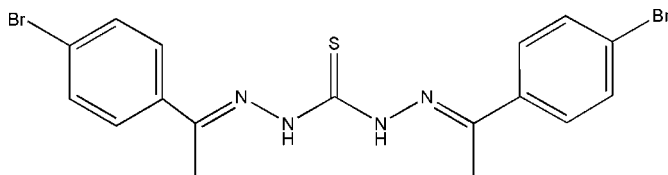
Received 30 March 2013; accepted 9 April 2013

 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.015$  Å;  $R$  factor = 0.073;  $wR$  factor = 0.214; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound,  $\text{C}_{17}\text{H}_{16}\text{Br}_2\text{N}_4\text{S}$ , contains two independent molecules in which the benzene rings form dihedral angles of  $20.0$  (1) and  $55.3$  (1)°. In the crystal, a pair of  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds link the two different independent molecules into a dimer.

## Related literature

For the crystal structures of related compounds, see: Feng *et al.* (2011); Zhao (2011); Schmitt *et al.* (2011).



## Experimental

### Crystal data

$\text{C}_{17}\text{H}_{16}\text{Br}_2\text{N}_4\text{S}$   
 $M_r = 468.22$   
 Triclinic,  $P\bar{1}$   
 $a = 11.5800$  (11) Å

$b = 13.6950$  (12) Å  
 $c = 14.2860$  (13) Å  
 $\alpha = 118.401$  (2)°  
 $\beta = 90.977$  (1)°

$\gamma = 108.404$  (1)°  
 $V = 1852.6$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

$\mu = 4.49$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.43 \times 0.37 \times 0.33$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.248$ ,  $T_{\max} = 0.319$

9457 measured reflections  
 6456 independent reflections  
 2949 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.081$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.073$   
 $wR(F^2) = 0.214$   
 $S = 0.96$   
 6456 reflections

438 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.90$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.33$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N5}-\text{H5B}\cdots\text{S1}$	0.86	2.71	3.551 (8)	168
$\text{N1}-\text{H1}\cdots\text{S2}$	0.86	2.69	3.551 (8)	174

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The author acknowledges financial support by Dongchang College, Liaocheng University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5398).

## References

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## supporting information

*Acta Cryst.* (2013). E69, o723 [https://doi.org/10.1107/S1600536813009720]

**1,5-Bis[1-(4-bromophenyl)ethylidene]thiocarbonohydrazide****Zhiqing Gao****S1. Comment**

In a continuation of our structural study of thiocarbonohydrazides (Feng *et al.*, 2011), we present here the title compound (I).

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in the related thiocarbonohydrazides (Feng *et al.*, 2011; Zhao, 2011; Schmitt *et al.*, 2011). The benzene rings C4—C9 and C12—C17 form a dihedral angle of 20.0 (1)°, while benzene rings C21—C26 and C29—C34 form a dihedral angle of 55.3 (1)°.

In the crystal, intermolecular N—H···S hydrogen bonds link two independent molecules into dimer (Fig. 1).

**S2. Experimental**

*p*-Br-Acetophenone (1.0 mmol) and thiocarbohydrazide (0.5 mmol) were mixed in 25 ml flash in the methanol. After 6 h stirring at 354 K, the resulting mixture was cooled to room temperature, and recrystallized from ethanol, and afforded the title compound as a crystalline solid.

**S3. Refinement**

All H atoms were placed in geometrically idealized positions (N—H 0.86 and C—H 0.93–0.96 Å) and treated as riding on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$  (C, N).

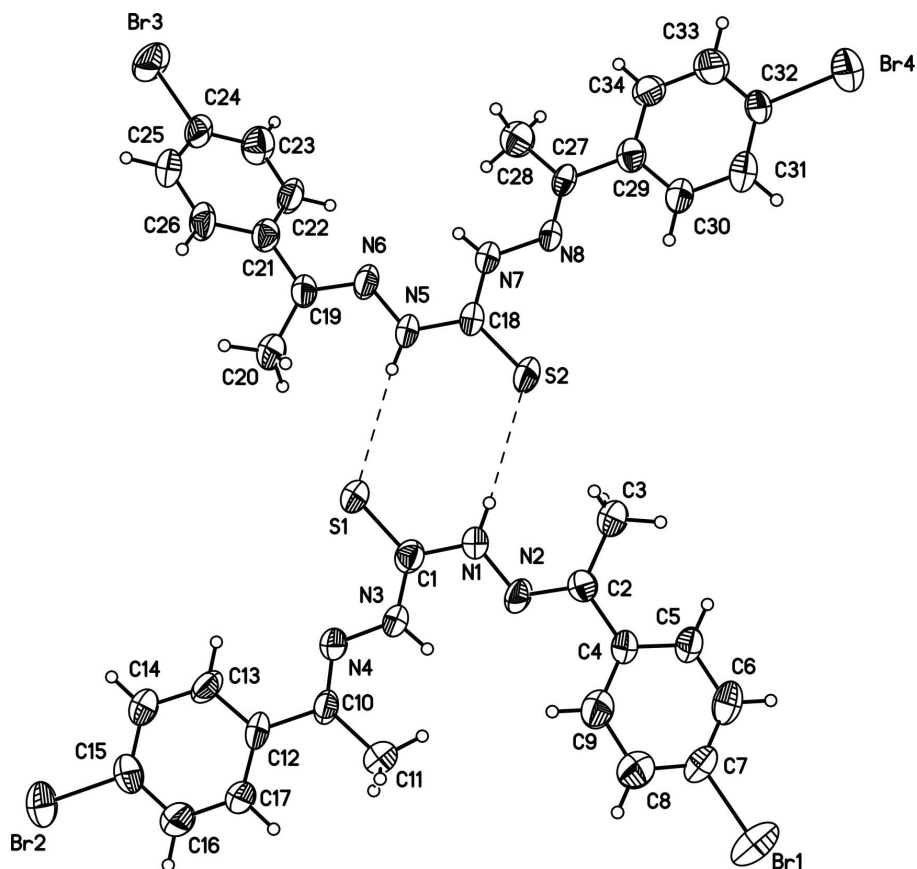


Figure 1

A hydrogen-bonded (dashed lines) dimer in the asymmetric unit of (I) showing the atomic numbering and 50% probability displacement ellipsoids

### 1,5-Bis[1-(4-bromophenyl)ethylidene]thiocarbonohydrazide

#### Crystal data

$C_{17}H_{16}Br_2N_4S$

$M_r = 468.22$

Triclinic,  $P\bar{1}$

$a = 11.5800$  (11) Å

$b = 13.6950$  (12) Å

$c = 14.2860$  (13) Å

$\alpha = 118.401$  (2)°

$\beta = 90.977$  (1)°

$\gamma = 108.404$  (1)°

$V = 1852.6$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 928$

$D_x = 1.679$  Mg m<sup>-3</sup>

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

Cell parameters from 2095 reflections

$\theta = 2.8$ – $21.2$ °

$\mu = 4.49$  mm<sup>-1</sup>

$T = 298$  K

Yellow, block

$0.43 \times 0.37 \times 0.33$  mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\omega$  scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.248$ ,  $T_{\max} = 0.319$

9457 measured reflections

6456 independent reflections

2949 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.081$   
 $\theta_{\text{max}} = 25.0^\circ$ ,  $\theta_{\text{min}} = 2.3^\circ$   
 $h = -7 \rightarrow 13$

$k = -16 \rightarrow 14$   
 $l = -16 \rightarrow 16$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.073$   
 $wR(F^2) = 0.214$   
 $S = 0.96$   
 6456 reflections  
 438 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  
 $w = 1/[\sigma^2(F_o^2) + (0.1033P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.90 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.33 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXL97* (Sheldrick,  
 2008),  $F_c^* = kFc^*[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0038 (8)

### Special details

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.86326 (12)	1.60584 (12)	1.59389 (9)	0.0846 (5)
Br2	1.15040 (11)	0.55332 (10)	0.95650 (10)	0.0669 (4)
Br3	0.32652 (11)	0.37660 (11)	-0.03711 (8)	0.0723 (4)
Br4	-0.09677 (12)	1.33393 (11)	0.64953 (10)	0.0787 (5)
N5	0.4538 (7)	0.8654 (6)	0.6079 (6)	0.045 (2)
H5B	0.4943	0.8559	0.6519	0.055*
N6	0.4306 (7)	0.7886 (6)	0.4978 (6)	0.046 (2)
N7	0.3534 (7)	0.9606 (6)	0.5655 (6)	0.049 (2)
H7	0.3550	0.9157	0.4987	0.058*
N8	0.2919 (7)	1.0377 (6)	0.5921 (6)	0.047 (2)
S2	0.4295 (3)	1.0494 (3)	0.7779 (2)	0.0688 (9)
C18	0.4121 (9)	0.9556 (8)	0.6457 (7)	0.045 (2)
C19	0.4609 (8)	0.6957 (8)	0.4612 (7)	0.041 (2)
C20	0.5183 (9)	0.6633 (9)	0.5305 (7)	0.056 (3)
H20A	0.6005	0.7214	0.5670	0.084*
H20B	0.5226	0.5860	0.4861	0.084*
H20C	0.4688	0.6615	0.5834	0.084*
C21	0.4303 (8)	0.6187 (8)	0.3412 (7)	0.042 (2)
C22	0.4345 (9)	0.6678 (8)	0.2735 (8)	0.052 (3)
H22	0.4588	0.7501	0.3053	0.062*

C23	0.4042 (9)	0.5988 (9)	0.1630 (8)	0.057 (3)
H23	0.4086	0.6328	0.1196	0.069*
C24	0.3668 (8)	0.4769 (9)	0.1180 (7)	0.047 (3)
C25	0.3645 (9)	0.4233 (9)	0.1799 (8)	0.051 (3)
H25	0.3407	0.3409	0.1470	0.061*
C26	0.3982 (9)	0.4952 (8)	0.2910 (8)	0.050 (3)
H26	0.3998	0.4610	0.3335	0.060*
C27	0.2443 (9)	1.0463 (7)	0.5156 (8)	0.044 (2)
C28	0.2551 (10)	0.9804 (9)	0.3973 (8)	0.061 (3)
H28A	0.3316	0.9665	0.3933	0.091*
H28B	0.2540	1.0277	0.3651	0.091*
H28C	0.1865	0.9053	0.3588	0.091*
C29	0.1686 (8)	1.1214 (8)	0.5468 (7)	0.041 (2)
C30	0.1683 (9)	1.1928 (8)	0.6561 (8)	0.051 (3)
H30	0.2209	1.1971	0.7091	0.061*
C31	0.0914 (10)	1.2570 (9)	0.6868 (9)	0.058 (3)
H31	0.0928	1.3050	0.7600	0.069*
C32	0.0137 (9)	1.2497 (8)	0.6096 (8)	0.048 (3)
C33	0.0121 (10)	1.1817 (9)	0.5017 (9)	0.061 (3)
H33	-0.0413	1.1780	0.4497	0.073*
C34	0.0898 (10)	1.1187 (9)	0.4703 (8)	0.053 (3)
H34	0.0896	1.0736	0.3968	0.064*
C1	0.6961 (9)	0.9711 (8)	0.9249 (7)	0.044 (2)
C2	0.6406 (8)	1.2301 (8)	1.1112 (7)	0.042 (2)
C3	0.5534 (10)	1.2427 (9)	1.0443 (8)	0.061 (3)
H3A	0.5938	1.2585	0.9922	0.091*
H3B	0.5283	1.3077	1.0904	0.091*
H3C	0.4816	1.1702	1.0071	0.091*
C4	0.6932 (8)	1.3211 (8)	1.2269 (7)	0.043 (2)
C5	0.6906 (8)	1.4327 (8)	1.2704 (7)	0.044 (2)
H5A	0.6540	1.4526	1.2269	0.053*
C6	0.7420 (9)	1.5178 (9)	1.3795 (8)	0.056 (3)
H6	0.7399	1.5939	1.4082	0.068*
C7	0.7958 (9)	1.4894 (9)	1.4448 (7)	0.051 (3)
C8	0.7975 (10)	1.3767 (10)	1.4055 (8)	0.066 (3)
H8	0.8305	1.3562	1.4504	0.079*
C9	0.7471 (10)	1.2936 (10)	1.2942 (8)	0.059 (3)
H9	0.7500	1.2177	1.2649	0.071*
C10	0.9075 (9)	0.9240 (8)	1.0604 (7)	0.042 (2)
C11	0.9352 (11)	1.0257 (10)	1.1749 (8)	0.076 (4)
H11A	0.9116	1.0871	1.1756	0.114*
H11B	1.0225	1.0573	1.2043	0.114*
H11C	0.8893	0.9976	1.2182	0.114*
C12	0.9696 (8)	0.8369 (8)	1.0347 (7)	0.042 (2)
C13	0.9539 (9)	0.7456 (8)	0.9292 (7)	0.050 (3)
H13	0.9045	0.7403	0.8736	0.060*
C14	1.0085 (10)	0.6628 (9)	0.9037 (8)	0.056 (3)
H14	0.9979	0.6037	0.8320	0.067*

C15	1.0793 (9)	0.6687 (9)	0.9861 (9)	0.050 (3)
C16	1.0998 (10)	0.7599 (10)	1.0913 (8)	0.062 (3)
H16	1.1509	0.7664	1.1465	0.074*
C17	1.0443 (10)	0.8407 (10)	1.1137 (8)	0.061 (3)
H17	1.0573	0.9010	1.1854	0.073*
S1	0.6625 (3)	0.8667 (2)	0.79389 (19)	0.0573 (8)
N1	0.6438 (7)	1.0560 (6)	0.9636 (6)	0.046 (2)
H1	0.5879	1.0546	0.9220	0.055*
N2	0.6838 (7)	1.1437 (7)	1.0710 (6)	0.045 (2)
N3	0.7716 (7)	0.9799 (7)	1.0024 (6)	0.051 (2)
H3	0.7833	1.0366	1.0681	0.061*
N4	0.8306 (7)	0.9031 (7)	0.9815 (6)	0.046 (2)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0993 (10)	0.0729 (10)	0.0402 (7)	0.0114 (7)	0.0123 (6)	0.0105 (6)
Br2	0.0741 (8)	0.0582 (8)	0.0797 (9)	0.0427 (6)	0.0312 (6)	0.0316 (6)
Br3	0.0858 (9)	0.0716 (9)	0.0357 (6)	0.0361 (7)	0.0156 (5)	0.0051 (6)
Br4	0.0866 (9)	0.0617 (9)	0.0857 (9)	0.0481 (7)	0.0081 (7)	0.0234 (7)
N5	0.060 (5)	0.032 (5)	0.037 (5)	0.026 (4)	0.007 (4)	0.007 (4)
N6	0.059 (5)	0.031 (5)	0.038 (5)	0.022 (4)	0.011 (4)	0.008 (4)
N7	0.064 (6)	0.038 (5)	0.036 (5)	0.030 (4)	0.004 (4)	0.006 (4)
N8	0.067 (6)	0.035 (5)	0.034 (5)	0.032 (4)	0.003 (4)	0.006 (4)
S2	0.112 (3)	0.0566 (19)	0.0339 (15)	0.0562 (17)	0.0061 (14)	0.0046 (13)
C18	0.056 (6)	0.031 (6)	0.042 (6)	0.023 (5)	0.006 (5)	0.009 (5)
C19	0.049 (6)	0.035 (6)	0.041 (6)	0.023 (5)	0.012 (4)	0.015 (5)
C20	0.074 (7)	0.052 (7)	0.039 (6)	0.037 (6)	0.013 (5)	0.011 (5)
C21	0.040 (6)	0.038 (6)	0.043 (6)	0.018 (5)	0.012 (4)	0.014 (5)
C22	0.070 (7)	0.031 (6)	0.043 (6)	0.020 (5)	0.007 (5)	0.009 (5)
C23	0.074 (8)	0.056 (8)	0.048 (7)	0.029 (6)	0.023 (5)	0.028 (6)
C24	0.037 (6)	0.044 (7)	0.043 (6)	0.023 (5)	0.013 (4)	0.006 (5)
C25	0.062 (7)	0.034 (6)	0.050 (7)	0.024 (5)	0.015 (5)	0.014 (5)
C26	0.057 (7)	0.025 (6)	0.062 (7)	0.014 (5)	0.010 (5)	0.019 (5)
C27	0.053 (6)	0.017 (5)	0.045 (6)	0.010 (4)	−0.002 (5)	0.006 (4)
C28	0.067 (7)	0.065 (8)	0.051 (7)	0.033 (6)	0.013 (5)	0.025 (6)
C29	0.044 (6)	0.030 (6)	0.049 (6)	0.011 (4)	0.011 (4)	0.021 (5)
C30	0.067 (7)	0.043 (6)	0.041 (6)	0.030 (5)	0.009 (5)	0.013 (5)
C31	0.071 (8)	0.039 (7)	0.056 (7)	0.029 (6)	0.015 (6)	0.014 (5)
C32	0.059 (7)	0.030 (6)	0.053 (7)	0.024 (5)	0.000 (5)	0.016 (5)
C33	0.072 (8)	0.042 (7)	0.066 (8)	0.021 (6)	−0.004 (6)	0.026 (6)
C34	0.071 (7)	0.037 (6)	0.045 (6)	0.018 (5)	−0.008 (5)	0.017 (5)
C1	0.051 (6)	0.032 (6)	0.041 (6)	0.013 (5)	0.007 (5)	0.015 (5)
C2	0.041 (6)	0.046 (6)	0.042 (6)	0.022 (5)	0.010 (4)	0.020 (5)
C3	0.076 (8)	0.068 (8)	0.039 (6)	0.046 (6)	0.017 (5)	0.016 (5)
C4	0.050 (6)	0.032 (6)	0.042 (6)	0.020 (5)	0.008 (4)	0.013 (5)
C5	0.056 (7)	0.033 (6)	0.041 (6)	0.020 (5)	0.015 (4)	0.015 (5)
C6	0.066 (7)	0.031 (6)	0.060 (7)	0.015 (5)	0.020 (6)	0.015 (5)

C7	0.063 (7)	0.040 (7)	0.034 (6)	0.014 (5)	0.012 (5)	0.009 (5)
C8	0.085 (9)	0.068 (9)	0.048 (7)	0.036 (7)	0.015 (6)	0.026 (6)
C9	0.075 (8)	0.057 (7)	0.049 (7)	0.034 (6)	0.019 (5)	0.021 (6)
C10	0.061 (7)	0.031 (6)	0.036 (6)	0.024 (5)	0.016 (5)	0.013 (5)
C11	0.105 (9)	0.067 (8)	0.043 (6)	0.050 (7)	-0.008 (6)	0.007 (6)
C12	0.044 (6)	0.027 (5)	0.045 (6)	0.016 (4)	0.015 (4)	0.009 (5)
C13	0.065 (7)	0.041 (6)	0.027 (5)	0.019 (5)	0.008 (4)	0.006 (5)
C14	0.073 (8)	0.049 (7)	0.041 (6)	0.034 (6)	0.016 (5)	0.011 (5)
C15	0.046 (6)	0.047 (7)	0.066 (7)	0.026 (5)	0.019 (5)	0.030 (6)
C16	0.073 (8)	0.064 (8)	0.043 (7)	0.037 (6)	0.007 (5)	0.016 (6)
C17	0.085 (8)	0.063 (8)	0.035 (6)	0.049 (6)	0.009 (5)	0.011 (5)
S1	0.081 (2)	0.0479 (17)	0.0348 (14)	0.0368 (15)	0.0041 (12)	0.0074 (12)
N1	0.055 (5)	0.038 (5)	0.041 (5)	0.026 (4)	0.005 (4)	0.013 (4)
N2	0.050 (5)	0.047 (5)	0.032 (4)	0.028 (4)	0.017 (4)	0.009 (4)
N3	0.074 (6)	0.037 (5)	0.035 (5)	0.030 (4)	0.002 (4)	0.006 (4)
N4	0.052 (5)	0.046 (5)	0.038 (5)	0.030 (4)	0.009 (4)	0.012 (4)

*Geometric parameters (Å, °)*

Br1—C7	1.902 (9)	C33—H33	0.9300
Br2—C15	1.885 (10)	C34—H34	0.9300
Br3—C24	1.918 (9)	C1—N3	1.333 (11)
Br4—C32	1.903 (10)	C1—N1	1.367 (11)
N5—C18	1.342 (11)	C1—S1	1.667 (9)
N5—N6	1.374 (10)	C2—N2	1.310 (11)
N5—H5B	0.8600	C2—C4	1.478 (12)
N6—C19	1.292 (11)	C2—C3	1.482 (12)
N7—C18	1.363 (11)	C3—H3A	0.9600
N7—N8	1.366 (10)	C3—H3B	0.9600
N7—H7	0.8600	C3—H3C	0.9600
N8—C27	1.285 (11)	C4—C5	1.360 (12)
S2—C18	1.666 (9)	C4—C9	1.388 (13)
C19—C21	1.484 (12)	C5—C6	1.394 (13)
C19—C20	1.484 (12)	C5—H5A	0.9300
C20—H20A	0.9600	C6—C7	1.373 (14)
C20—H20B	0.9600	C6—H6	0.9300
C20—H20C	0.9600	C7—C8	1.376 (14)
C21—C26	1.397 (12)	C8—C9	1.412 (13)
C21—C22	1.410 (13)	C8—H8	0.9300
C22—C23	1.364 (13)	C9—H9	0.9300
C22—H22	0.9300	C10—N4	1.282 (11)
C23—C24	1.378 (13)	C10—C12	1.486 (12)
C23—H23	0.9300	C10—C11	1.501 (13)
C24—C25	1.388 (13)	C11—H11A	0.9600
C25—C26	1.375 (13)	C11—H11B	0.9600
C25—H25	0.9300	C11—H11C	0.9600
C26—H26	0.9300	C12—C17	1.382 (13)
C27—C29	1.474 (13)	C12—C13	1.386 (12)

C27—C28	1.522 (13)	C13—C14	1.374 (13)
C28—H28A	0.9600	C13—H13	0.9300
C28—H28B	0.9600	C14—C15	1.378 (13)
C28—H28C	0.9600	C14—H14	0.9300
C29—C34	1.391 (12)	C15—C16	1.374 (13)
C29—C30	1.395 (13)	C16—C17	1.363 (14)
C30—C31	1.378 (13)	C16—H16	0.9300
C30—H30	0.9300	C17—H17	0.9300
C31—C32	1.357 (13)	N1—N2	1.372 (10)
C31—H31	0.9300	N1—H1	0.8600
C32—C33	1.366 (14)	N3—N4	1.350 (10)
C33—C34	1.374 (14)	N3—H3	0.8600
C18—N5—N6	118.9 (8)	N3—C1—N1	113.2 (8)
C18—N5—H5B	120.5	N3—C1—S1	125.1 (8)
N6—N5—H5B	120.5	N1—C1—S1	121.7 (7)
C19—N6—N5	119.3 (8)	N2—C2—C4	115.2 (8)
C18—N7—N8	119.5 (8)	N2—C2—C3	123.0 (8)
C18—N7—H7	120.3	C4—C2—C3	121.5 (8)
N8—N7—H7	120.3	C2—C3—H3A	109.5
C27—N8—N7	118.1 (8)	C2—C3—H3B	109.5
N5—C18—N7	113.3 (8)	H3A—C3—H3B	109.5
N5—C18—S2	122.5 (7)	C2—C3—H3C	109.5
N7—C18—S2	124.2 (7)	H3A—C3—H3C	109.5
N6—C19—C21	114.5 (8)	H3B—C3—H3C	109.5
N6—C19—C20	124.5 (8)	C5—C4—C9	118.4 (9)
C21—C19—C20	121.0 (8)	C5—C4—C2	121.7 (9)
C19—C20—H20A	109.5	C9—C4—C2	120.0 (9)
C19—C20—H20B	109.5	C4—C5—C6	120.8 (9)
H20A—C20—H20B	109.5	C4—C5—H5A	119.6
C19—C20—H20C	109.5	C6—C5—H5A	119.6
H20A—C20—H20C	109.5	C7—C6—C5	120.1 (9)
H20B—C20—H20C	109.5	C7—C6—H6	119.9
C26—C21—C22	117.5 (9)	C5—C6—H6	119.9
C26—C21—C19	121.3 (9)	C6—C7—C8	121.3 (9)
C22—C21—C19	121.1 (8)	C6—C7—Br1	119.5 (8)
C23—C22—C21	122.3 (9)	C8—C7—Br1	119.1 (8)
C23—C22—H22	118.8	C7—C8—C9	117.0 (10)
C21—C22—H22	118.8	C7—C8—H8	121.5
C22—C23—C24	117.7 (10)	C9—C8—H8	121.5
C22—C23—H23	121.2	C4—C9—C8	122.3 (10)
C24—C23—H23	121.2	C4—C9—H9	118.9
C23—C24—C25	122.8 (9)	C8—C9—H9	118.9
C23—C24—Br3	119.1 (8)	N4—C10—C12	116.0 (8)
C25—C24—Br3	117.9 (7)	N4—C10—C11	125.2 (9)
C26—C25—C24	118.3 (9)	C12—C10—C11	118.7 (8)
C26—C25—H25	120.9	C10—C11—H11A	109.5
C24—C25—H25	120.9	C10—C11—H11B	109.5



C25—C26—C21	121.3 (9)	H11A—C11—H11B	109.5
C25—C26—H26	119.4	C10—C11—H11C	109.5
C21—C26—H26	119.4	H11A—C11—H11C	109.5
N8—C27—C29	115.9 (9)	H11B—C11—H11C	109.5
N8—C27—C28	125.0 (9)	C17—C12—C13	116.2 (9)
C29—C27—C28	119.0 (8)	C17—C12—C10	122.4 (8)
C27—C28—H28A	109.5	C13—C12—C10	121.4 (9)
C27—C28—H28B	109.5	C14—C13—C12	122.5 (9)
H28A—C28—H28B	109.5	C14—C13—H13	118.8
C27—C28—H28C	109.5	C12—C13—H13	118.8
H28A—C28—H28C	109.5	C13—C14—C15	119.0 (10)
H28B—C28—H28C	109.5	C13—C14—H14	120.5
C34—C29—C30	117.6 (9)	C15—C14—H14	120.5
C34—C29—C27	122.3 (9)	C16—C15—C14	120.2 (9)
C30—C29—C27	119.9 (8)	C16—C15—Br2	119.1 (8)
C31—C30—C29	121.0 (9)	C14—C15—Br2	120.8 (8)
C31—C30—H30	119.5	C17—C16—C15	119.3 (10)
C29—C30—H30	119.5	C17—C16—H16	120.4
C32—C31—C30	119.6 (10)	C15—C16—H16	120.4
C32—C31—H31	120.2	C16—C17—C12	122.9 (10)
C30—C31—H31	120.2	C16—C17—H17	118.6
C31—C32—C33	121.1 (10)	C12—C17—H17	118.6
C31—C32—Br4	120.5 (8)	C1—N1—N2	117.6 (7)
C33—C32—Br4	118.4 (7)	C1—N1—H1	121.2
C32—C33—C34	119.7 (9)	N2—N1—H1	121.2
C32—C33—H33	120.1	C2—N2—N1	120.2 (8)
C34—C33—H33	120.1	C1—N3—N4	122.5 (8)
C33—C34—C29	120.9 (10)	C1—N3—H3	118.8
C33—C34—H34	119.5	N4—N3—H3	118.8
C29—C34—H34	119.5	C10—N4—N3	117.5 (8)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5B $\cdots$ S1	0.86	2.71	3.551 (8)	168
N1—H1 $\cdots$ S2	0.86	2.69	3.551 (8)	174