

## 2,3-Dihydrobenz[4,5]imidazo[2,1-*b*]thiazole

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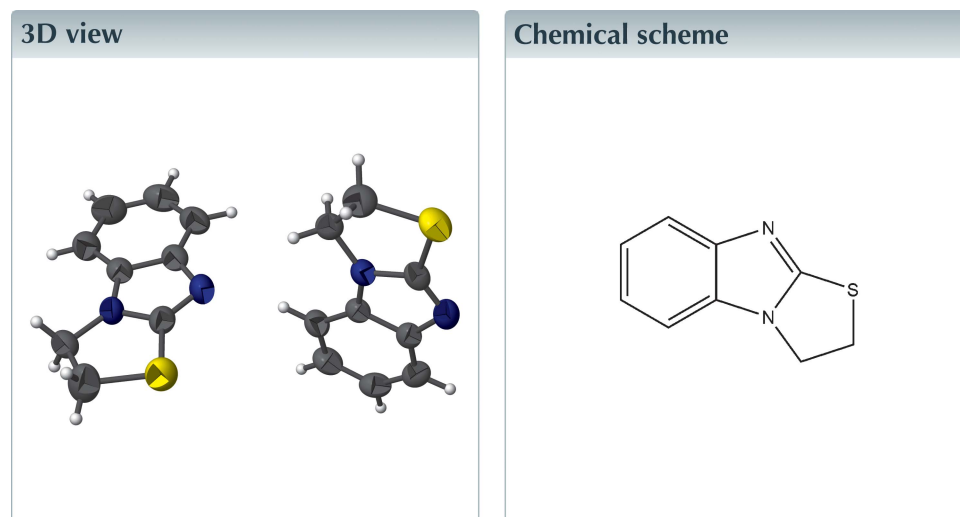
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Keywords: crystal structure; thiazole; benzoimidazole; hydrogen bonding;  $\pi$ - $\pi$  stacking; C—H $\cdots$  $\pi$  interactions.

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Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>S, consists of two independent molecules (*A* and *B*) differing in the conformation of the thiazole ring: twisted for molecule *A* and planar for molecule *B*. In the crystal, molecules stack along the *c* axis in alternating *A* and *B* layers. Within the layers, molecules are linked by C—H $\cdots$  $\pi$  interactions, and inversion-related *B* molecules are linked by offset  $\pi$ - $\pi$  interactions [inter-centroid distance = 3.716 (1) Å]. The two molecules are also linked by a C—H $\cdots$ N hydrogen bond, which results finally in the formation of a three-dimensional structure.

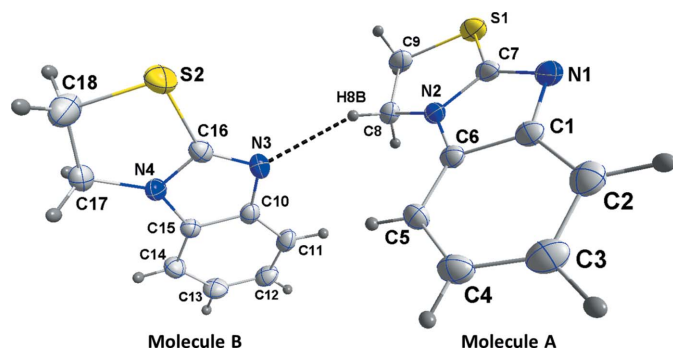


### Structure description

An enormous variety of thiazolo[3,2-*a*]benzimidazoles, with unique pharmaceutical and medicinal applications, have been reported (Piskin *et al.*, 2009; Le Sann *et al.*, 2006). As a continuation of our research devoted to the development of benzimidazole derivatives (El Bakri *et al.* 2016), the title compound was prepared and characterized by single-crystal X-ray diffraction.

The asymmetric unit of the title compound, Fig. 1, consists of two independent molecules (*A* and *B*), differing in the conformation of the five-membered thiazole ring. In molecule *A*, the ring (S1/N2/C7–C9) has a twisted conformation on the C8–C9 bond, while in molecule *B* the ring (S2/N4/C16–C18) is planar (r.m.s. deviation = 0.035 Å).

In the crystal, molecules stack along the *c* axis in alternating *A* and *B* layers (Fig. 2). Within the layers, molecules are linked by C—H $\cdots$  $\pi$  interactions (Fig. 2 and Table 1), and inversion-related *B* molecules are linked by offset  $\pi$ - $\pi$  interactions [*Cg*7 $\cdots$ *Cg*9<sup>i</sup> = 3.716 (1) Å; *Cg*7 and *Cg*9 are the centroids of the S2/N4/C16–C18 and C10–C15 rings, respectively; interplanar distance = 3.638 (1) Å, slippage = 0.763 Å; symmetry code: (i)

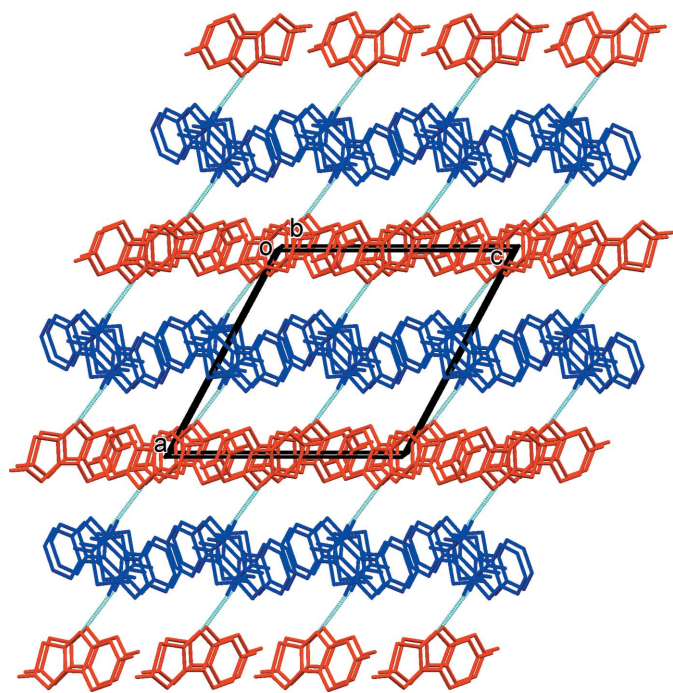


**Figure 1**  
The molecular structures of the two independent molecules (*A* and *B*) of the title compound, showing the atom labelling and 25% probability displacement ellipsoids. The intermolecular C—H···N hydrogen bond is shown as a dashed line (see Table 1).

$-x, -y + 1, -z + 1$ ]. The two molecules are also linked by a C—H···N hydrogen bond (Table 1), which results finally in the formation of a three-dimensional structure (Fig. 2).

### Synthesis and crystallization

To a solution of benzimidazole-2-thione (1 g, 7 mmol) in 20 ml of dimethylformamide, were added potassium bicarbonate (1.93 g, 14 mmol), bromotetrabutylammonium (0.1 mmol) and 1,2-dibromoethane (3.5 mmol). The reaction mixture was stirred at room temperature for 4 h. After evaporation of the solvent under reduced pressure, the residue was chromato-



**Figure 2**  
A view along the *b* axis of the crystal packing of the title compound (*A* molecules shown in blue and *B* molecules in red). The C—H···N hydrogen bonds (see Table 1) are shown as dashed lines, and for clarity only the H atoms involved in the intermolecular interactions have been included.

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

*Cg*3, *Cg*7 and *Cg*9 are the centroids of the C1–C6, S2/N4/C16–C18 and C10–C15 rings, respectively.

<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>
C8—H8 <i>B</i> ···N3	0.92 (2)	2.62 (2)	3.464 (2)	154 (2)
C8—H8 <i>A</i> ··· <i>Cg</i> 3 <sup>i</sup>	0.97 (2)	2.65 (2)	3.543 (2)	154 (2)
C9—H9 <i>A</i> ··· <i>Cg</i> 3 <sup>ii</sup>	0.94 (2)	2.99 (2)	3.661 (3)	129 (2)
C12—H12··· <i>Cg</i> 7 <sup>iii</sup>	0.94 (2)	2.94 (2)	3.838 (2)	161 (2)
C18—H18 <i>A</i> ··· <i>Cg</i> 9 <sup>iv</sup>	0.85 (3)	2.90 (3)	3.471 (4)	126 (3)

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> S
<i>M<sub>r</sub></i>	176.23
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	298
<i>a, b, c</i> (Å)	12.7440 (8), 11.4820 (7), 12.8707 (8)
$\beta$ (°)	118.234 (1)
<i>V</i> (Å <sup>3</sup> )	1659.25 (18)
<i>Z</i>	8
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.33
Crystal size (mm)	0.38 × 0.22 × 0.06
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2016)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.87, 0.98
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	15538, 4244, 2702
<i>R<sub>int</sub></i>	0.036
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.685
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, 0.134, 1.02
No. of reflections	4244
No. of parameters	281
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.27, -0.25

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012, *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

graphed on silica gel (hexane/ethyl acetate: 80/20), giving a solid product. Colourless plate-like crystals were obtained by recrystallization from ethanol solution to afford the title compound in 80% yield.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

### Acknowledgements

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## full crystallographic data

*IUCrData* (2016). **1**, x161948 [<https://doi.org/10.1107/S2414314616019489>]

2,3-Dihydrobenz[4,5]imidazo[2,1-*b*]thiazole

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2,3-Dihydrobenz[4,5]imidazo[2,1-*b*]thiazole*Crystal data*

$C_9H_8N_2S$

$M_r = 176.23$

Monoclinic,  $P2_1/c$

$a = 12.7440$  (8) Å

$b = 11.4820$  (7) Å

$c = 12.8707$  (8) Å

$\beta = 118.234$  (1)°

$V = 1659.25$  (18) Å<sup>3</sup>

$Z = 8$

$F(000) = 736$

$D_x = 1.411$  Mg m<sup>-3</sup>

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

Cell parameters from 4421 reflections

$\theta = 2.5$ – $25.4$ °

$\mu = 0.33$  mm<sup>-1</sup>

$T = 298$  K

Plate, colourless

$0.38 \times 0.22 \times 0.06$  mm

*Data collection*

Bruker SMART APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3333 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2016)

$T_{\min} = 0.87$ ,  $T_{\max} = 0.98$

15538 measured reflections

4244 independent reflections

2702 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 29.1$ °,  $\theta_{\min} = 1.8$ °

$h = -17 \rightarrow 17$

$k = -15 \rightarrow 15$

$l = -16 \rightarrow 17$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.134$

$S = 1.02$

4244 reflections

281 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2]$

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

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

$\Delta\rho_{\max} = 0.27$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.25$  e Å<sup>-3</sup>

*Special details*

**Experimental.** The diffraction data were collected in three sets of 363 frames ( $0.5^\circ$  width in  $\omega$ ) at  $\varphi = 0, 120$  and  $240^\circ$ . A scan time of 40 sec/frame was used.

**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 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.60928 (5)	0.83270 (4)	0.50755 (5)	0.06186 (19)
N1	0.67791 (13)	0.67804 (12)	0.69522 (13)	0.0494 (4)
N2	0.48777 (12)	0.67647 (11)	0.55018 (12)	0.0423 (3)
C1	0.61392 (15)	0.59028 (14)	0.71572 (15)	0.0433 (4)
C2	0.65137 (19)	0.51054 (16)	0.80769 (17)	0.0530 (5)
H2	0.7323 (17)	0.5100 (17)	0.8657 (17)	0.067 (6)*
C3	0.5701 (2)	0.43030 (17)	0.80575 (18)	0.0571 (5)
H3	0.5961 (19)	0.375 (2)	0.8645 (19)	0.076 (6)*
C4	0.4535 (2)	0.42874 (17)	0.71608 (19)	0.0585 (5)
H4	0.3984 (17)	0.3748 (19)	0.7162 (17)	0.067 (6)*
C5	0.41276 (17)	0.50738 (16)	0.62405 (17)	0.0503 (4)
H5	0.3330 (18)	0.5108 (18)	0.5642 (16)	0.064 (6)*
C6	0.49469 (14)	0.58756 (13)	0.62549 (14)	0.0408 (4)
C7	0.59884 (15)	0.72369 (15)	0.59596 (15)	0.0442 (4)
C8	0.40008 (17)	0.71382 (17)	0.43372 (16)	0.0489 (4)
H8A	0.3903 (15)	0.6550 (16)	0.3759 (15)	0.047 (5)*
H8B	0.3277 (17)	0.7257 (16)	0.4307 (15)	0.054 (5)*
C9	0.4497 (2)	0.8251 (2)	0.4088 (2)	0.0637 (6)
H9A	0.435 (2)	0.8278 (18)	0.330 (2)	0.080 (7)*
H9B	0.4210 (19)	0.895 (2)	0.4243 (19)	0.084 (8)*
S2	0.09273 (5)	0.81657 (5)	0.59932 (5)	0.06511 (19)
N3	0.14754 (13)	0.66410 (13)	0.46357 (14)	0.0531 (4)
N4	-0.03893 (13)	0.66826 (12)	0.43993 (13)	0.0447 (3)
C10	0.07636 (16)	0.58368 (15)	0.37754 (16)	0.0480 (4)
C11	0.1060 (2)	0.50724 (18)	0.31224 (19)	0.0605 (5)
H11	0.1862 (18)	0.5015 (17)	0.3240 (16)	0.066 (6)*
C12	0.0190 (2)	0.43527 (18)	0.2334 (2)	0.0686 (6)
H12	0.0374 (18)	0.384 (2)	0.1871 (18)	0.073 (6)*
C13	-0.0963 (2)	0.43830 (19)	0.2175 (2)	0.0716 (6)
H13	-0.152 (2)	0.389 (2)	0.166 (2)	0.091 (8)*
C14	-0.12870 (19)	0.51306 (18)	0.28185 (18)	0.0591 (5)
H14	-0.203 (2)	0.512 (2)	0.2730 (19)	0.084 (7)*
C15	-0.04071 (15)	0.58468 (14)	0.36185 (15)	0.0442 (4)

C16	0.07387 (15)	0.71029 (15)	0.49625 (15)	0.0469 (4)
C17	-0.12433 (18)	0.71370 (19)	0.47270 (19)	0.0520 (5)
H17A	-0.1465 (16)	0.6577 (16)	0.5092 (16)	0.053 (5)*
H17B	-0.1870 (19)	0.740 (2)	0.4091 (19)	0.075 (7)*
C18	-0.0634 (2)	0.8086 (3)	0.5617 (3)	0.0783 (7)
H18A	-0.070 (3)	0.805 (3)	0.625 (3)	0.131 (13)*
H18B	-0.094 (3)	0.885 (3)	0.530 (3)	0.140 (13)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0674 (4)	0.0543 (3)	0.0757 (4)	-0.0089 (2)	0.0435 (3)	0.0056 (2)
N1	0.0439 (8)	0.0468 (8)	0.0566 (9)	-0.0006 (6)	0.0230 (8)	-0.0052 (7)
N2	0.0413 (8)	0.0416 (8)	0.0472 (8)	-0.0001 (6)	0.0235 (7)	0.0012 (6)
C1	0.0447 (10)	0.0410 (8)	0.0463 (9)	0.0037 (7)	0.0234 (8)	-0.0053 (7)
C2	0.0562 (12)	0.0519 (11)	0.0466 (10)	0.0112 (9)	0.0208 (9)	-0.0023 (8)
C3	0.0768 (15)	0.0488 (11)	0.0510 (11)	0.0088 (10)	0.0347 (11)	0.0075 (9)
C4	0.0698 (14)	0.0514 (11)	0.0667 (13)	-0.0033 (10)	0.0425 (12)	0.0069 (9)
C5	0.0467 (11)	0.0521 (10)	0.0566 (11)	-0.0026 (8)	0.0282 (9)	0.0031 (9)
C6	0.0442 (9)	0.0388 (8)	0.0444 (9)	0.0026 (7)	0.0250 (8)	-0.0015 (7)
C7	0.0458 (10)	0.0389 (9)	0.0549 (11)	-0.0022 (7)	0.0295 (9)	-0.0065 (7)
C8	0.0495 (11)	0.0529 (11)	0.0459 (10)	0.0042 (9)	0.0238 (9)	0.0050 (9)
C9	0.0703 (15)	0.0566 (13)	0.0652 (14)	0.0022 (10)	0.0329 (12)	0.0119 (10)
S2	0.0623 (4)	0.0667 (4)	0.0651 (4)	-0.0156 (2)	0.0291 (3)	-0.0188 (2)
N3	0.0410 (9)	0.0622 (10)	0.0572 (9)	-0.0010 (7)	0.0242 (8)	-0.0005 (7)
N4	0.0386 (8)	0.0468 (8)	0.0481 (8)	0.0000 (6)	0.0200 (7)	-0.0020 (6)
C10	0.0489 (10)	0.0487 (10)	0.0493 (10)	0.0088 (8)	0.0255 (9)	0.0107 (8)
C11	0.0673 (14)	0.0630 (12)	0.0626 (13)	0.0156 (11)	0.0400 (12)	0.0100 (10)
C12	0.0960 (18)	0.0571 (12)	0.0657 (14)	0.0089 (12)	0.0487 (14)	-0.0015 (11)
C13	0.0914 (18)	0.0595 (13)	0.0663 (14)	-0.0141 (12)	0.0393 (14)	-0.0150 (11)
C14	0.0571 (13)	0.0608 (12)	0.0614 (12)	-0.0111 (10)	0.0297 (11)	-0.0076 (10)
C15	0.0477 (10)	0.0408 (8)	0.0465 (9)	0.0007 (7)	0.0242 (8)	0.0027 (7)
C16	0.0427 (10)	0.0480 (9)	0.0467 (10)	-0.0032 (8)	0.0184 (8)	0.0017 (8)
C17	0.0496 (11)	0.0583 (11)	0.0543 (12)	0.0018 (9)	0.0298 (10)	0.0017 (10)
C18	0.0618 (14)	0.0847 (18)	0.0860 (18)	0.0015 (13)	0.0330 (14)	-0.0303 (15)

*Geometric parameters (Å, °)*

S1—C7	1.7385 (18)	S2—C16	1.7336 (18)
S1—C9	1.821 (3)	S2—C18	1.813 (3)
N1—C7	1.305 (2)	N3—C16	1.309 (2)
N1—C1	1.398 (2)	N3—C10	1.397 (2)
N2—C7	1.362 (2)	N4—C16	1.356 (2)
N2—C6	1.381 (2)	N4—C15	1.382 (2)
N2—C8	1.447 (2)	N4—C17	1.438 (2)
C1—C2	1.390 (3)	C10—C11	1.385 (3)
C1—C6	1.410 (2)	C10—C15	1.408 (2)
C2—C3	1.378 (3)	C11—C12	1.370 (3)

C2—H2	0.945 (19)	C11—H11	0.961 (19)
C3—C4	1.384 (3)	C12—C13	1.385 (3)
C3—H3	0.92 (2)	C12—H12	0.94 (2)
C4—C5	1.381 (3)	C13—C14	1.385 (3)
C4—H4	0.94 (2)	C13—H13	0.90 (2)
C5—C6	1.386 (2)	C14—C15	1.379 (3)
C5—H5	0.942 (19)	C14—H14	0.90 (2)
C8—C9	1.525 (3)	C17—C18	1.503 (3)
C8—H8A	0.968 (18)	C17—H17A	0.917 (19)
C8—H8B	0.915 (19)	C17—H17B	0.88 (2)
C9—H9A	0.94 (2)	C18—H18A	0.85 (3)
C9—H9B	0.94 (2)	C18—H18B	0.97 (3)
C7—S1—C9	90.94 (9)	C16—S2—C18	91.29 (10)
C7—N1—C1	103.00 (14)	C16—N3—C10	103.12 (14)
C7—N2—C6	106.40 (14)	C16—N4—C15	106.52 (14)
C7—N2—C8	117.73 (14)	C16—N4—C17	118.16 (15)
C6—N2—C8	135.01 (15)	C15—N4—C17	135.30 (15)
C2—C1—N1	129.76 (17)	C11—C10—N3	129.68 (18)
C2—C1—C6	119.26 (17)	C11—C10—C15	119.51 (18)
N1—C1—C6	110.98 (15)	N3—C10—C15	110.80 (15)
C3—C2—C1	118.20 (19)	C12—C11—C10	118.3 (2)
C3—C2—H2	122.7 (12)	C12—C11—H11	120.2 (12)
C1—C2—H2	119.0 (12)	C10—C11—H11	121.5 (12)
C2—C3—C4	121.65 (19)	C11—C12—C13	121.7 (2)
C2—C3—H3	118.0 (14)	C11—C12—H12	119.2 (13)
C4—C3—H3	120.3 (14)	C13—C12—H12	119.1 (13)
C5—C4—C3	121.78 (19)	C12—C13—C14	121.5 (2)
C5—C4—H4	117.1 (13)	C12—C13—H13	119.9 (17)
C3—C4—H4	121.1 (13)	C14—C13—H13	118.5 (17)
C4—C5—C6	116.60 (18)	C15—C14—C13	116.7 (2)
C4—C5—H5	123.5 (12)	C15—C14—H14	122.5 (15)
C6—C5—H5	119.8 (12)	C13—C14—H14	120.7 (15)
N2—C6—C5	133.16 (16)	C14—C15—N4	133.23 (17)
N2—C6—C1	104.34 (14)	C14—C15—C10	122.31 (17)
C5—C6—C1	122.50 (16)	N4—C15—C10	104.46 (15)
N1—C7—N2	115.25 (15)	N3—C16—N4	115.10 (16)
N1—C7—S1	131.83 (14)	N3—C16—S2	132.09 (14)
N2—C7—S1	112.90 (13)	N4—C16—S2	112.81 (13)
N2—C8—C9	105.81 (16)	N4—C17—C18	107.23 (17)
N2—C8—H8A	110.2 (11)	N4—C17—H17A	110.8 (12)
C9—C8—H8A	109.8 (10)	C18—C17—H17A	107.0 (12)
N2—C8—H8B	110.9 (11)	N4—C17—H17B	109.3 (14)
C9—C8—H8B	112.1 (12)	C18—C17—H17B	111.7 (15)
H8A—C8—H8B	108.1 (15)	H17A—C17—H17B	110.8 (18)
C8—C9—S1	109.29 (15)	C17—C18—S2	110.27 (16)
C8—C9—H9A	111.2 (14)	C17—C18—H18A	116 (2)
S1—C9—H9A	109.9 (14)	S2—C18—H18A	109 (2)

C8—C9—H9B	115.4 (14)	C17—C18—H18B	112 (2)
S1—C9—H9B	103.2 (13)	S2—C18—H18B	104.2 (19)
H9A—C9—H9B	107.5 (19)	H18A—C18—H18B	104 (3)
C7—N1—C1—C2	179.00 (17)	C16—N3—C10—C11	-178.96 (19)
C7—N1—C1—C6	-0.63 (17)	C16—N3—C10—C15	-0.18 (19)
N1—C1—C2—C3	-178.60 (17)	N3—C10—C11—C12	179.12 (18)
C6—C1—C2—C3	1.0 (2)	C15—C10—C11—C12	0.4 (3)
C1—C2—C3—C4	-0.8 (3)	C10—C11—C12—C13	0.5 (3)
C2—C3—C4—C5	0.0 (3)	C11—C12—C13—C14	-1.0 (4)
C3—C4—C5—C6	0.4 (3)	C12—C13—C14—C15	0.4 (3)
C7—N2—C6—C5	-178.18 (18)	C13—C14—C15—N4	-179.87 (19)
C8—N2—C6—C5	-9.5 (3)	C13—C14—C15—C10	0.6 (3)
C7—N2—C6—C1	1.27 (16)	C16—N4—C15—C14	180.0 (2)
C8—N2—C6—C1	169.95 (17)	C17—N4—C15—C14	1.7 (3)
C4—C5—C6—N2	179.21 (17)	C16—N4—C15—C10	-0.44 (18)
C4—C5—C6—C1	-0.2 (3)	C17—N4—C15—C10	-178.74 (19)
C2—C1—C6—N2	179.90 (14)	C11—C10—C15—C14	-1.0 (3)
N1—C1—C6—N2	-0.42 (17)	N3—C10—C15—C14	-179.95 (17)
C2—C1—C6—C5	-0.6 (2)	C11—C10—C15—N4	179.32 (16)
N1—C1—C6—C5	179.10 (15)	N3—C10—C15—N4	0.40 (18)
C1—N1—C7—N2	1.54 (18)	C10—N3—C16—N4	-0.1 (2)
C1—N1—C7—S1	-176.53 (14)	C10—N3—C16—S2	179.86 (15)
C6—N2—C7—N1	-1.88 (19)	C15—N4—C16—N3	0.4 (2)
C8—N2—C7—N1	-172.86 (15)	C17—N4—C16—N3	179.02 (16)
C6—N2—C7—S1	176.57 (11)	C15—N4—C16—S2	-179.61 (11)
C8—N2—C7—S1	5.59 (19)	C17—N4—C16—S2	-1.0 (2)
C9—S1—C7—N1	-176.19 (18)	C18—S2—C16—N3	178.1 (2)
C9—S1—C7—N2	5.70 (14)	C18—S2—C16—N4	-1.92 (17)
C7—N2—C8—C9	-16.1 (2)	C16—N4—C17—C18	4.0 (3)
C6—N2—C8—C9	176.18 (18)	C15—N4—C17—C18	-177.8 (2)
N2—C8—C9—S1	18.9 (2)	N4—C17—C18—S2	-5.1 (3)
C7—S1—C9—C8	-14.46 (17)	C16—S2—C18—C17	4.1 (2)

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

Cg3, Cg7 and Cg9 are the centroids of the C1–C6, S2/N4/C16–C18 and C10–C15 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8B $\cdots$ N3	0.92 (2)	2.62 (2)	3.464 (2)	154 (2)
C8—H8A $\cdots$ Cg3 <sup>i</sup>	0.97 (2)	2.65 (2)	3.543 (2)	154 (2)
C9—H9A $\cdots$ Cg3 <sup>ii</sup>	0.94 (2)	2.99 (2)	3.661 (3)	129 (2)
C12—H12 $\cdots$ Cg7 <sup>iii</sup>	0.94 (2)	2.94 (2)	3.838 (2)	161 (2)
C18—H18A $\cdots$ Cg9 <sup>iv</sup>	0.85 (3)	2.90 (3)	3.471 (4)	126 (3)

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