

## 6-Methylbenzo[d]thiazol-2-amine

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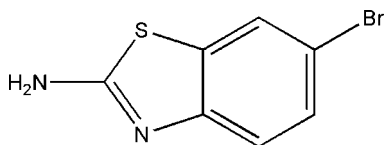
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.084; data-to-parameter ratio = 14.5.

The title compound,  $\text{C}_8\text{H}_8\text{N}_2\text{S}$ , crystallizes with two almost identical molecules in the asymmetric unit. In the crystal structure, it is remarkable that only three of the four amino H atoms form classical hydrogen bonds. The fourth H atom is involved in an  $\text{N}-\text{H}\cdots\pi$  interaction.

## Related literature

For information on the biological and medical applications of aminobenzothiazoles, see: Dessi & Ben-Asi (1993); Benavides *et al.* (1985); Hutchinson *et al.* (2002); El-Sherbeny (2000); Delmas *et al.* (2002); Láková *et al.* (1991). For their pesticidal and antimicrobial activities, see: Kaufmann (1935); Pattan *et al.* (2002). For a related structure see Jai-nhuknan *et al.* (1997).



## Experimental

## Crystal data

$\text{C}_8\text{H}_8\text{N}_2\text{S}$	$\gamma = 96.592$ (10)°
$M_r = 164.22$	$V = 786.55$ (16) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 4$
$a = 5.8174$ (6) Å	Mo $K\alpha$ radiation
$b = 9.1150$ (12) Å	$\mu = 0.34$ mm <sup>-1</sup>
$c = 15.0897$ (17) Å	$T = 173$ (2) K
$\alpha = 93.167$ (9)°	$0.33 \times 0.32 \times 0.29$ mm
$\beta = 97.233$ (10)°	

## Data collection

Stoe IPDSII two-circle diffractometer	9276 measured reflections
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	3154 independent reflections
$T_{\min} = 0.896$ , $T_{\max} = 0.908$	2900 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.041$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.084$	
$S = 1.03$	
3154 reflections	$\Delta\rho_{\text{max}} = 0.29$ e Å <sup>-3</sup>
218 parameters	$\Delta\rho_{\text{min}} = -0.27$ e Å <sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

 $C_g$  is the centroid of the benzene ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N2A}$	0.86 (2)	2.18 (2)	3.0211 (18)	163.4 (18)
$\text{N1}-\text{H1B}\cdots\text{N1A}^i$	0.92 (2)	2.43 (2)	3.2264 (18)	144.9 (18)
$\text{N1A}-\text{H1C}\cdots\text{N2}^{ii}$	0.93 (2)	2.15 (2)	3.0356 (18)	158.3 (17)
$\text{N1A}-\text{H1D}\cdots C_g^{iii}$	0.93 (2)	2.42	3.420	166

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP in SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2362).

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**supplementary materials**

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## 6-Methylbenzo[d]thiazol-2-amine

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### Comment

Various 2-aminobenzothiazoles find several applications in medicinal chemistry, drug discovery and development of therapeutic agents for the treatment of a variety of diseases. Riluzole [6-(trifluoromethoxy)-2-benzothiazolamine] interferes with glutamate neurotransmission, antagonizes the release of acetylcholine induced by *N*-methyl-D-aspartate and blocks the increase in cyclic guanosine monophosphate levels in the cerebellar cortex induced by glutamate (Dessi & Ben-Asi, 1993). Additionally it possesses anticonvulsant and neuroprotective effects (Benavides *et al.*, 1985). Phenyl substituted benzothiazoles show very intensive antitumor activity (Hutchinson *et al.*, 2002) and condensed pyrimido[2,1-*b*]benzothiazole and benzothiazolo[2,3-*b*]quinazolines exert antiviral activity (El-Sherbeny 2000). Bis-substituted amidino benzothiazoles are potential anti-HIV agents (Delmas *et al.*, 2002). 6-Ethoxy-2-amino benzothiazole is a typical strong local anesthetic (Lácová *et al.*, 1991) and acyl derivatives of 4-chloro-2-aminobenzothiazole possess pesticidal activities (Kaufmann, 1935). 2-Substituted 6-nitro and 6-amino benzothiazoles and fluorobenzothiazoles show antimicrobial activity (Pattan *et al.*, 2002).

The title compound crystallizes with two almost identical molecules in the asymmetric unit. A least-squares fit overlaying all non-H atoms gives an r.m.s. deviation of 0.062 Å. The crystal packing is stabilized by N—H···N hydrogen bonds and N—H··· $\pi$  interactions (Table 1). It is remarkable that only three of the four amino H atoms form classic hydrogen bonds. The fourth one is involved in an N—H··· $\pi$  interaction [N1A—H1D···Cg<sup>i</sup>,  $i = 1 - x, 1 - y, 1 - z$  where Cg is the centroid of the C2···C7 benzene ring; H1D···Cg<sup>i</sup> 2.42 (2) Å, N1A—H1D···Cg<sup>i</sup> 167 (2)°].

### Experimental

A mixture of *p*-toluidine (3 g, 0.03 mol) and potassium thiocyanate (11.6 g, 0.12 mol) in AcOH (45 ml) was stirred at 20° C for 10 minutes. A solution of bromine (1.5 ml, 0.03 mol) in AcOH (20 ml) was added over 20 min. and the reaction mixture was stirred for 21 h at room temperature. The reaction mixture was poured into cold NH<sub>4</sub>OH (90 ml) and extracted with EtOAc. The organic phase was washed with water, dried filtered and evaporated. The crude product obtained was recrystallized using ethanol as solvent. Yield 76%; MP 135–137 ° C; IR (cm<sup>-1</sup>) 1602 (C=C), 1532 (C—N), 2725 (C—S), 3396 (N—H), 1635 (C=N); <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  2.51 (3H,s, ArCH<sub>3</sub>), 5.43 (1H, bs, NH), 7.46 (1H, d, J=8.7 Hz), 7.10 (1H, d, J=2.4 Hz), 6.91 (1H, dd, J=8.7, 2.4 Hz); EIMS m/e: 164 (37%)

### Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [ $U(H) = 1.2 U_{eq}(C)$  or  $U(H) = 1.5 U_{eq}(C_{methyl})$ ] using a riding model with C—H = 0.95 Å or C<sub>methyl</sub>—H = 0.98 Å. The amino H atoms were refined freely.

## Figures

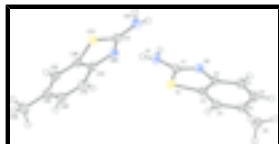


Fig. 1. Molecular structure of the two unique molecules of the title compound with anisotropic displacement ellipsoids drawn at the 50% probability level

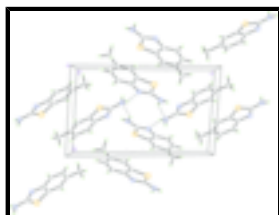


Fig. 2. Crystal packing for (I) with hydrogen bonds shown as dashed lines.

## 6-Methylbenzo[d]thiazol-2-amine

### Crystal data

$C_8H_8N_2S$	$Z = 4$
$M_r = 164.22$	$F_{000} = 344$
Triclinic, $P\bar{1}$	$D_x = 1.387 \text{ Mg m}^{-3}$
Hall symbol: $-P\ 1$	Mo $K\alpha$ radiation
$a = 5.8174 (6) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 9.1150 (12) \text{ \AA}$	Cell parameters from 8290 reflections
$c = 15.0897 (17) \text{ \AA}$	$\theta = 3.6\text{--}26.4^\circ$
$\alpha = 93.167 (9)^\circ$	$\mu = 0.34 \text{ mm}^{-1}$
$\beta = 97.233 (10)^\circ$	$T = 173 (2) \text{ K}$
$\gamma = 96.592 (10)^\circ$	Block, light brown
$V = 786.55 (16) \text{ \AA}^3$	$0.33 \times 0.32 \times 0.29 \text{ mm}$

### Data collection

Stoe IPDSII two-circle diffractometer	3154 independent reflections
Radiation source: fine-focus sealed tube	2900 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.041$
$T = 173(2) \text{ K}$	$\theta_{\text{max}} = 26.3^\circ$
$\omega$ scans	$\theta_{\text{min}} = 3.6^\circ$
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.896$ , $T_{\text{max}} = 0.908$	$k = -11 \rightarrow 11$
9276 measured reflections	$l = -18 \rightarrow 17$

### Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
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Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.032$$

$$wR(F^2) = 0.084$$

$$S = 1.03$$

3154 reflections

218 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.307P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL97 (Sheldrick, 1997),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.020 (4)

### 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  $F^2 > 2\sigma(F^2)$  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	0.23118 (6)	0.21396 (4)	0.55557 (2)	0.02484 (12)
C1	-0.0260 (2)	0.30261 (15)	0.53845 (9)	0.0197 (3)
N1	-0.0894 (2)	0.37788 (15)	0.60907 (9)	0.0255 (3)
H1A	0.011 (4)	0.403 (2)	0.6562 (15)	0.036 (5)*
H1B	-0.216 (4)	0.428 (2)	0.5959 (14)	0.044 (6)*
N2	-0.1407 (2)	0.28530 (13)	0.45774 (8)	0.0213 (3)
C2	-0.0301 (2)	0.19589 (15)	0.40221 (9)	0.0196 (3)
C3	0.1735 (2)	0.14371 (15)	0.44353 (9)	0.0200 (3)
C4	0.3022 (2)	0.05398 (16)	0.39606 (10)	0.0229 (3)
H4	0.4390	0.0204	0.4251	0.027*
C5	0.2273 (2)	0.01417 (15)	0.30541 (10)	0.0220 (3)
C6	0.0287 (3)	0.06973 (17)	0.26387 (10)	0.0260 (3)
H6	-0.0199	0.0452	0.2018	0.031*
C7	-0.0993 (3)	0.15994 (17)	0.31098 (10)	0.0253 (3)
H7	-0.2326	0.1966	0.2812	0.030*
C8	0.3577 (3)	-0.08893 (17)	0.25373 (10)	0.0270 (3)
H8A	0.5262	-0.0616	0.2703	0.041*
H8B	0.3166	-0.0807	0.1893	0.041*
H8C	0.3146	-0.1911	0.2682	0.041*
S1A	0.76943 (6)	0.53815 (4)	0.81495 (2)	0.02363 (12)

## supplementary materials

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C1A	0.5205 (2)	0.52790 (15)	0.73255 (9)	0.0201 (3)
N1A	0.5394 (2)	0.59802 (15)	0.65586 (9)	0.0250 (3)
H1C	0.401 (4)	0.607 (2)	0.6190 (14)	0.034 (5)*
H1D	0.650 (4)	0.666 (2)	0.6577 (14)	0.038 (5)*
N2A	0.3341 (2)	0.44627 (13)	0.74930 (8)	0.0207 (3)
C2A	0.3787 (2)	0.38328 (15)	0.83140 (9)	0.0198 (3)
C3A	0.6062 (2)	0.41915 (15)	0.87741 (9)	0.0208 (3)
C4A	0.6777 (3)	0.36119 (17)	0.95848 (10)	0.0245 (3)
H4A	0.8325	0.3868	0.9879	0.029*
C5A	0.5178 (3)	0.26475 (17)	0.99576 (10)	0.0267 (3)
C6A	0.2901 (3)	0.23073 (17)	0.95093 (11)	0.0284 (3)
H6A	0.1809	0.1664	0.9768	0.034*
C7A	0.2183 (3)	0.28812 (17)	0.86957 (10)	0.0257 (3)
H7A	0.0630	0.2630	0.8405	0.031*
C8A	0.5920 (3)	0.1975 (2)	1.08303 (12)	0.0377 (4)
H8A1	0.6289	0.0969	1.0702	0.057*
H8A2	0.4647	0.1941	1.1199	0.057*
H8A3	0.7305	0.2581	1.1153	0.057*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0252 (2)	0.0312 (2)	0.01881 (19)	0.01339 (14)	-0.00278 (13)	0.00009 (14)
C1	0.0184 (6)	0.0198 (7)	0.0215 (7)	0.0040 (5)	0.0024 (5)	0.0044 (5)
N1	0.0235 (6)	0.0314 (7)	0.0221 (6)	0.0096 (5)	0.0006 (5)	-0.0013 (5)
N2	0.0194 (6)	0.0234 (6)	0.0217 (6)	0.0066 (5)	0.0006 (4)	0.0016 (5)
C2	0.0193 (6)	0.0188 (6)	0.0204 (7)	0.0031 (5)	0.0008 (5)	0.0017 (5)
C3	0.0209 (6)	0.0201 (7)	0.0189 (7)	0.0037 (5)	0.0000 (5)	0.0034 (5)
C4	0.0237 (7)	0.0221 (7)	0.0237 (7)	0.0081 (5)	0.0013 (5)	0.0027 (6)
C5	0.0234 (7)	0.0187 (7)	0.0242 (7)	0.0028 (5)	0.0044 (5)	0.0009 (5)
C6	0.0283 (7)	0.0286 (8)	0.0196 (7)	0.0047 (6)	-0.0017 (6)	-0.0021 (6)
C7	0.0235 (7)	0.0300 (8)	0.0219 (7)	0.0085 (6)	-0.0039 (5)	0.0014 (6)
C8	0.0279 (7)	0.0263 (7)	0.0272 (8)	0.0059 (6)	0.0047 (6)	-0.0028 (6)
S1A	0.01826 (18)	0.0280 (2)	0.0238 (2)	0.00143 (13)	-0.00034 (13)	0.00397 (14)
C1A	0.0199 (6)	0.0211 (7)	0.0201 (7)	0.0084 (5)	0.0015 (5)	0.0001 (5)
N1A	0.0233 (6)	0.0275 (7)	0.0257 (7)	0.0059 (5)	0.0033 (5)	0.0080 (5)
N2A	0.0193 (5)	0.0233 (6)	0.0202 (6)	0.0063 (4)	0.0013 (4)	0.0017 (5)
C2A	0.0212 (6)	0.0195 (7)	0.0193 (7)	0.0069 (5)	0.0018 (5)	-0.0003 (5)
C3A	0.0218 (7)	0.0204 (7)	0.0206 (7)	0.0054 (5)	0.0029 (5)	-0.0012 (5)
C4A	0.0261 (7)	0.0263 (7)	0.0210 (7)	0.0084 (6)	-0.0013 (5)	-0.0004 (6)
C5A	0.0368 (8)	0.0246 (7)	0.0207 (7)	0.0112 (6)	0.0044 (6)	0.0018 (6)
C6A	0.0315 (8)	0.0257 (8)	0.0303 (8)	0.0047 (6)	0.0098 (6)	0.0065 (6)
C7A	0.0212 (7)	0.0268 (8)	0.0291 (8)	0.0033 (5)	0.0029 (6)	0.0025 (6)
C8A	0.0494 (10)	0.0391 (10)	0.0270 (8)	0.0139 (8)	0.0036 (7)	0.0101 (7)

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

S1—C3	1.7518 (14)	S1A—C3A	1.7517 (15)
S1—C1	1.7778 (14)	S1A—C1A	1.7760 (14)

C1—N2	1.3052 (19)	C1A—N2A	1.3029 (19)
C1—N1	1.3488 (19)	C1A—N1A	1.3629 (19)
N1—H1A	0.86 (2)	N1A—H1C	0.93 (2)
N1—H1B	0.92 (2)	N1A—H1D	0.84 (2)
N2—C2	1.4002 (17)	N2A—C2A	1.4013 (18)
C2—C7	1.395 (2)	C2A—C7A	1.400 (2)
C2—C3	1.4125 (19)	C2A—C3A	1.4089 (19)
C3—C4	1.3974 (19)	C3A—C4A	1.394 (2)
C4—C5	1.397 (2)	C4A—C5A	1.397 (2)
C4—H4	0.9500	C4A—H4A	0.9500
C5—C6	1.404 (2)	C5A—C6A	1.402 (2)
C5—C8	1.5159 (19)	C5A—C8A	1.518 (2)
C6—C7	1.395 (2)	C6A—C7A	1.395 (2)
C6—H6	0.9500	C6A—H6A	0.9500
C7—H7	0.9500	C7A—H7A	0.9500
C8—H8A	0.9800	C8A—H8A1	0.9800
C8—H8B	0.9800	C8A—H8A2	0.9800
C8—H8C	0.9800	C8A—H8A3	0.9800
C3—S1—C1	88.54 (6)	C3A—S1A—C1A	88.76 (7)
N2—C1—N1	125.62 (13)	N2A—C1A—N1A	124.90 (13)
N2—C1—S1	116.12 (10)	N2A—C1A—S1A	116.06 (11)
N1—C1—S1	118.24 (11)	N1A—C1A—S1A	118.96 (11)
C1—N1—H1A	119.7 (13)	C1A—N1A—H1C	117.3 (12)
C1—N1—H1B	115.0 (13)	C1A—N1A—H1D	116.5 (15)
H1A—N1—H1B	121.3 (19)	H1C—N1A—H1D	117.9 (19)
C1—N2—C2	110.33 (11)	C1A—N2A—C2A	110.18 (12)
C7—C2—N2	125.72 (13)	C7A—C2A—N2A	125.48 (13)
C7—C2—C3	118.66 (13)	C7A—C2A—C3A	118.57 (13)
N2—C2—C3	115.58 (12)	N2A—C2A—C3A	115.94 (12)
C4—C3—C2	121.75 (13)	C4A—C3A—C2A	122.32 (14)
C4—C3—S1	128.82 (11)	C4A—C3A—S1A	128.60 (11)
C2—C3—S1	109.40 (10)	C2A—C3A—S1A	109.06 (11)
C5—C4—C3	119.27 (13)	C3A—C4A—C5A	118.89 (14)
C5—C4—H4	120.4	C3A—C4A—H4A	120.6
C3—C4—H4	120.4	C5A—C4A—H4A	120.6
C4—C5—C6	118.85 (13)	C4A—C5A—C6A	118.96 (14)
C4—C5—C8	120.14 (13)	C4A—C5A—C8A	120.08 (15)
C6—C5—C8	121.01 (13)	C6A—C5A—C8A	120.96 (15)
C7—C6—C5	121.98 (14)	C7A—C6A—C5A	122.26 (14)
C7—C6—H6	119.0	C7A—C6A—H6A	118.9
C5—C6—H6	119.0	C5A—C6A—H6A	118.9
C2—C7—C6	119.43 (13)	C6A—C7A—C2A	118.98 (14)
C2—C7—H7	120.3	C6A—C7A—H7A	120.5
C6—C7—H7	120.3	C2A—C7A—H7A	120.5
C5—C8—H8A	109.5	C5A—C8A—H8A1	109.5
C5—C8—H8B	109.5	C5A—C8A—H8A2	109.5
H8A—C8—H8B	109.5	H8A1—C8A—H8A2	109.5
C5—C8—H8C	109.5	C5A—C8A—H8A3	109.5
H8A—C8—H8C	109.5	H8A1—C8A—H8A3	109.5

## supplementary materials

H8B—C8—H8C	109.5	H8A2—C8A—H8A3	109.5
C3—S1—C1—N2	-1.37 (12)	C3A—S1A—C1A—N2A	0.59 (11)
C3—S1—C1—N1	176.96 (12)	C3A—S1A—C1A—N1A	-176.27 (12)
N1—C1—N2—C2	-177.47 (14)	N1A—C1A—N2A—C2A	176.22 (12)
S1—C1—N2—C2	0.73 (16)	S1A—C1A—N2A—C2A	-0.43 (15)
C1—N2—C2—C7	-177.03 (14)	C1A—N2A—C2A—C7A	-179.20 (13)
C1—N2—C2—C3	0.56 (17)	C1A—N2A—C2A—C3A	-0.03 (17)
C7—C2—C3—C4	-1.9 (2)	C7A—C2A—C3A—C4A	1.2 (2)
N2—C2—C3—C4	-179.71 (13)	N2A—C2A—C3A—C4A	-178.06 (12)
C7—C2—C3—S1	176.22 (11)	C7A—C2A—C3A—S1A	179.69 (10)
N2—C2—C3—S1	-1.55 (15)	N2A—C2A—C3A—S1A	0.46 (15)
C1—S1—C3—C4	179.52 (14)	C1A—S1A—C3A—C4A	177.85 (14)
C1—S1—C3—C2	1.54 (11)	C1A—S1A—C3A—C2A	-0.55 (10)
C2—C3—C4—C5	-0.2 (2)	C2A—C3A—C4A—C5A	-0.4 (2)
S1—C3—C4—C5	-178.01 (11)	S1A—C3A—C4A—C5A	-178.58 (11)
C3—C4—C5—C6	2.1 (2)	C3A—C4A—C5A—C6A	-0.7 (2)
C3—C4—C5—C8	-177.12 (13)	C3A—C4A—C5A—C8A	178.78 (13)
C4—C5—C6—C7	-1.8 (2)	C4A—C5A—C6A—C7A	1.0 (2)
C8—C5—C6—C7	177.38 (14)	C8A—C5A—C6A—C7A	-178.48 (15)
N2—C2—C7—C6	179.74 (14)	C5A—C6A—C7A—C2A	-0.2 (2)
C3—C2—C7—C6	2.2 (2)	N2A—C2A—C7A—C6A	178.28 (13)
C5—C6—C7—C2	-0.4 (2)	C3A—C2A—C7A—C6A	-0.9 (2)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ N2A	0.86 (2)	2.18 (2)	3.0211 (18)	163.4 (18)
N1—H1B $\cdots$ N1A <sup>i</sup>	0.92 (2)	2.43 (2)	3.2264 (18)	144.9 (18)
N1A—H1C $\cdots$ N2 <sup>ii</sup>	0.93 (2)	2.15 (2)	3.0356 (18)	158.3 (17)
N1A—H1D $\cdots$ Cg <sup>iii</sup>	0.93	2.42	3.240	166

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



Fig. 1

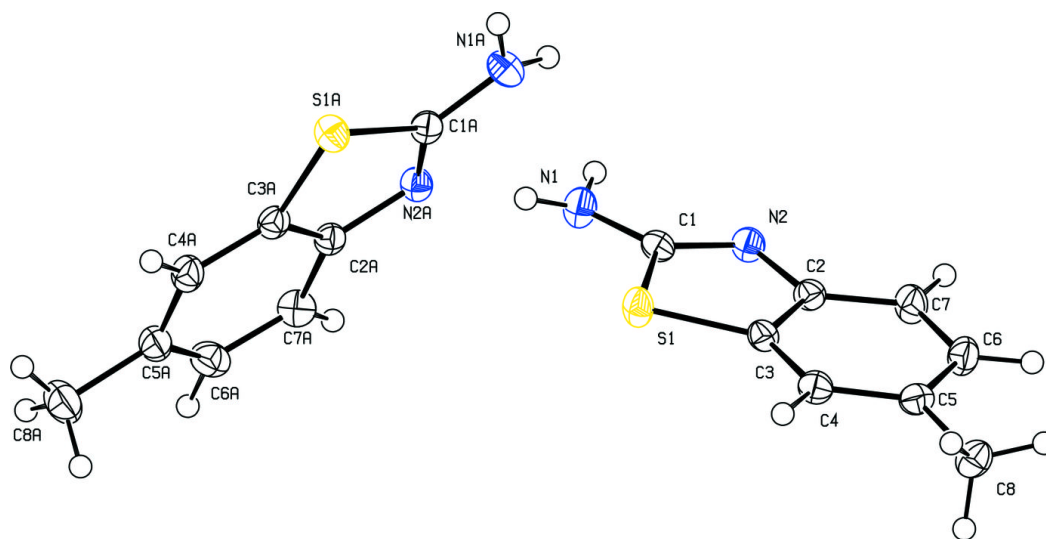


Fig. 2

