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# 2-(1,3-Benzothiazol-2-ylsulfanyl)-1-phenylethanone

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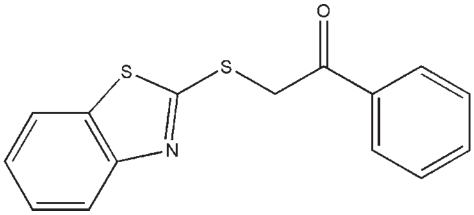
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.027; $wR$ factor = 0.068; data-to-parameter ratio = 21.7.

In the molecule of the title compound, $C_{15}H_{11}NOS_2$, the 1,3-benzothiazole ring is oriented at a dihedral angle of 6.61 (6)° with respect to the phenyl ring. In the crystal structure, intermolecular C—H⋯O interactions link the molecules in a herring-bone arrangement along the $b$ axis and $\pi$–$\pi$ contacts between the thiazole and phenyl rings [centroid–centroid distance = 3.851 (1) Å] may further stabilize the structure.

## Related literature

For applications of the title compound in organic synthesis, see: Marco *et al.* (1995); Fuju *et al.* (1988); Ni *et al.* (2006); Grossert *et al.* (1984); Oishi *et al.* (1988); Antane *et al.* (2004). For its biological activity, see: Padmavathi *et al.* (2008).



## Experimental

### *Crystal data*

$C_{15}H_{11}NOS_2$
$M_r$ = 285.37
Orthorhombic, $P2_12_12_1$
$a$ = 5.1060 (1) Å
$b$ = 14.6220 (3) Å
$c$ = 17.3920 (4) Å
$V$ = 1298.49 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.40 mm$^{-1}$
$T$ = 295 K
0.45 × 0.32 × 0.17 mm

### *Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.841, $T_{max}$ = 0.935
14309 measured reflections
3734 independent reflections
3576 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.068
$S$ = 1.07
3734 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Absolute structure: Flack (1983), 1550 Friedel pairs
Flack parameter: 0.01 (5)

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C2—H2$A$⋯O1$^{i}$ | 0.93 | 2.51 | 3.2299 (17) | 135 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2004); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

We thank the University of Isfahan and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2756).

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# supporting information

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## 2-(1,3-Benzothiazol-2-ylsulfanyl)-1-phenylethanone

**Hossein Loghmani-Khouzani, Dariush Hajiheidari, Ward T. Robinson, Noorsaadah Abdul Rahman and Reza Kia**

### S1. Comment

2-(Benzo[d]thiaazol-2-ylthio)-1-phenylethanone is of great importance in organic synthesis and $\beta$-keto-sulfones are a very important group of intermediates as they are precursors for Michael and Knoevenagel reactions and are used in the preparation of acetylenes, allenes, chalcones, vinyl sulfones, polyfunctionalized 4H-pyrans and ketones (Marco *et al.*, 1995; Fuju *et al.*, 1988; Ni *et al.*, 2006). In addition, $\beta$-keto-sulfones can be converted into optically active $\beta$-hydroxy-sulfones, halomethyl and dihalomethyl sulfones. Halomethyl and dihalomethyl sulfones are very good $\alpha$-carbanion stabilizing substituents and precursors for the preparation of alkenes, aziridines, epoxides and $\beta$-hydroxy-sulfones. Haloalkyl sulfones are useful in preventing aquatic organisms from attaching to fishing nets and ship hulls (Grossert *et al.*, 1984; Oishi *et al.*, 1988; Antane *et al.*, 2004). They also possess other biological properties such as herbicidal, bactericidal antifungal and insecticidal. Recently sulfone-linked heterocycles were prepared and have been showed antimicrobial activity (Padmavathi *et al.*, 2008). We prepared the title compound as a precursor for the synthesis of gem-difluoromethylene-containing heterocycle, and reported herein its crystal structure.

In the molecule of the title compound, (Fig. 1), the benzothiazole ring is oriented with respect to the phenyl ring at a dihedral angle of 6.61 (6)°. In the crystal structure, intermolecular C-H···O interactions (Table 1) link the molecules in herringbone mode along the b axis (Fig. 2), in which they may be effective in the stabilization of the structure. The $\pi$–$\pi$ contact between the thiazole and phenyl rings, Cg1—Cg2$^{i}$, [symmetry code: (i) x - 1, y, z, where Cg1 and Cg2 are centroids of the rings (S1/N1/C1/C6/C7) and (C1-C6), respectively] may further stabilize the structure, with centroid-centroid distance of 3.851 (1) Å.

### S2. Experimental

For the preparation of the title compound, sodium carbonate (4.5 mmol) was added to a stirred solution of 2-mercaptobenzothiazole (3 mmol) in ethanol (15 ml) and water (15 ml) and stirred at room temperature for 30 min. $\alpha$-Bromoacetophenone (3 mmol) was added to the reaction mixture and stirring was continued for 1h. The reaction was monitored by TLC and after 60 min showed the complete disappearance of the starting material. The reaction mixture was poured into HCl (1M, 100 ml) containing crushed ice (50 g). The product was filtered under vacuum and filtrate washed with ice-cold ethanol (10 ml) and water (10 ml). Recrystalization from petrol ether and filtration gave the title compound (m.p. 387-389 K). $^{1}$H NMR (400 MHz; $CDCl_3$): 8.15-7.75 (m, 4H), 7.55-7.32 (m, 5H), 5.10 (s, 2H). $^{13}$C NMR (126 MHz; $CDCl_3$): 194.2 (C=O), 162.1, 151.8, 135.3, 134.2, 131.1, 126.7, 126.5, 124.7, 124.1, 119.8, 119.6, 37.5. Anal. Calcd. for CHNS: C, 63.13; H, 3.89; N, 4.91. Found: C, 63.07; H, 3.86; N, 4.93.

## S3. Refinement

H atoms were positioned geometrically with C-H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

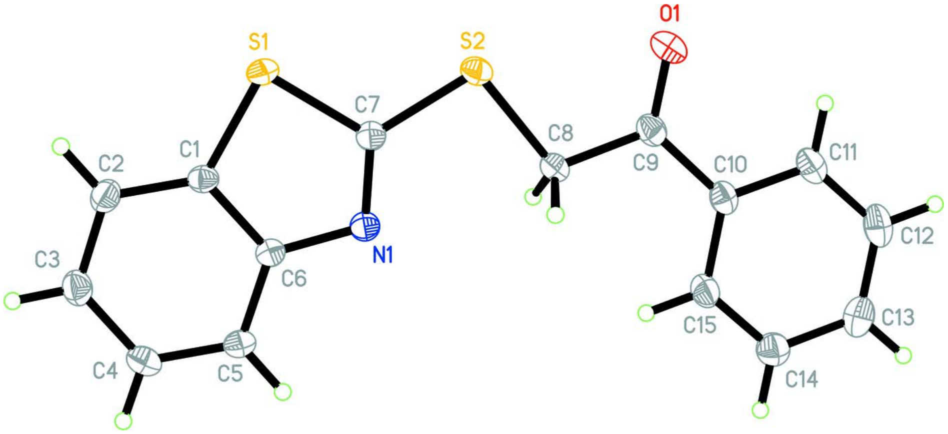

**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level

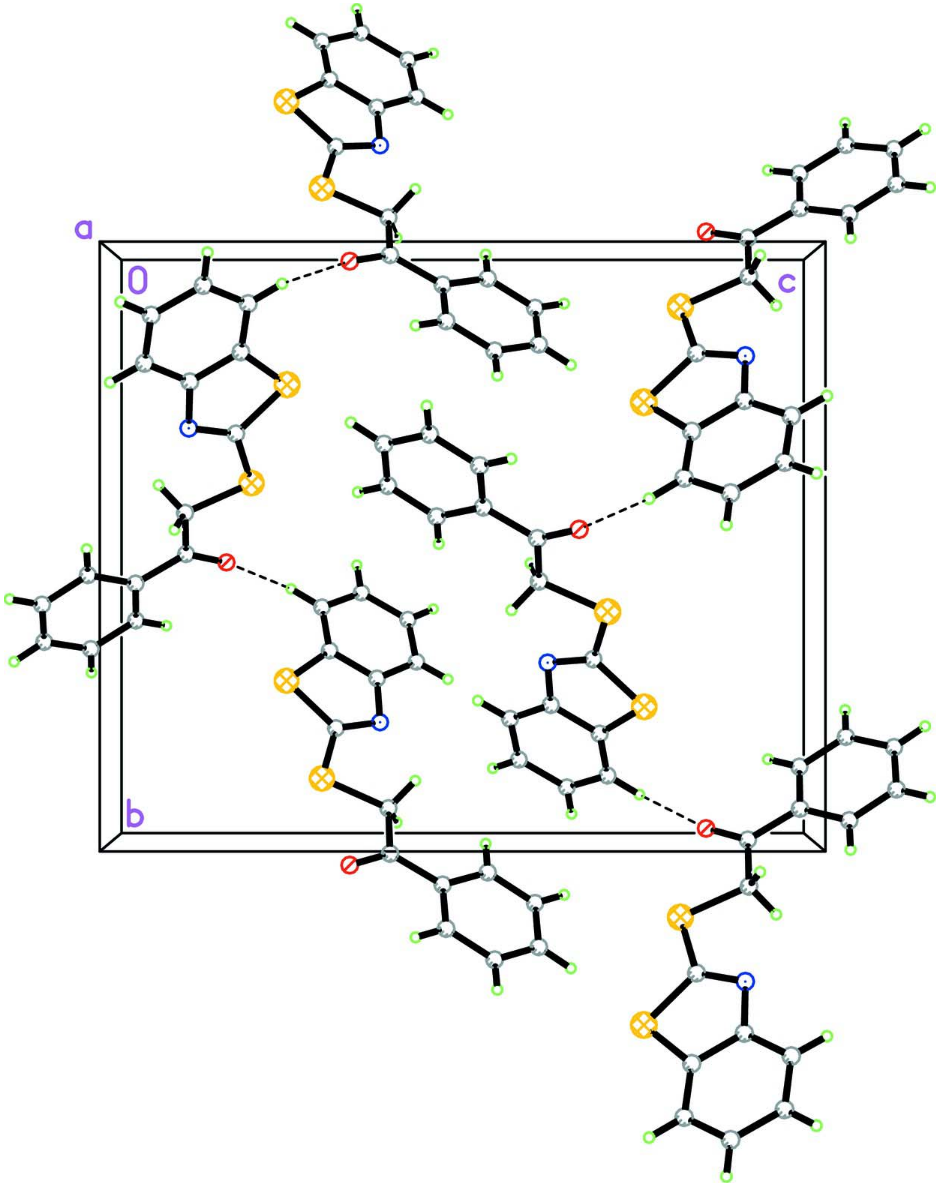

**Figure 2**

A partial packing diagram. Hydrogen bonds are shown as dashed lines.

## 2-(1,3-Benzothiazol-2-ylsulfanyl)-1-phenylethanone

*Crystal data*

$C_{15}H_{11}NOS_2$
$M_r = 285.37$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.1060$ (1) Å
$b = 14.6220$ (3) Å
$c = 17.3920$ (4) Å
$V = 1298.49$ (5) Å$^3$
$Z = 4$
$F(000) = 592$

$D_x = 1.460$ Mg m$^{-3}$
Melting point: 388 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8370 reflections
$\theta = 2.3$–30.5°
$\mu = 0.40$ mm$^{-1}$
$T = 295$ K
Block, pale-yellow
0.45 × 0.32 × 0.17 mm

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 14309 measured reflections |
| Radiation source: fine-focus sealed tube | 3734 independent reflections |
| Graphite monochromator | 3576 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{\text{int}} = 0.024$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $\theta_{\text{max}} = 30.0°$, $\theta_{\text{min}} = 2.7°$ |
| $T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.935$ | $h = -7 \rightarrow 6$ |
| | $k = -20 \rightarrow 20$ |
| | $l = -24 \rightarrow 24$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.027$ | $w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.1348P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.068$ | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| $S = 1.07$ | $\Delta\rho_{\text{max}} = 0.31$ e Å$^{-3}$ |
| 3734 reflections | $\Delta\rho_{\text{min}} = -0.16$ e Å$^{-3}$ |
| 172 parameters | Absolute structure: Flack (1983), 1550 Friedel pairs |
| 0 restraints | Absolute structure parameter: 0.01 (5) |
| Primary atom site location: structure-invariant direct methods | |
| Secondary atom site location: difference Fourier map | |

*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 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 $F^2$ > 2sigma($F^2$) 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{\text{iso}}$*/$U_{\text{eq}}$ |
|---|---|---|---|---|
| S1 | 0.32503 (6) | 0.26829 (2) | 0.744608 (17) | 0.02052 (8) |
| S2 | 0.01546 (7) | 0.10723 (2) | 0.799872 (17) | 0.02062 (8) |
| O1 | −0.3471 (2) | −0.02751 (8) | 0.84299 (6) | 0.0341 (3) |
| N1 | 0.3955 (2) | 0.19530 (7) | 0.87979 (6) | 0.0178 (2) |
| C1 | 0.5575 (2) | 0.31781 (8) | 0.80443 (7) | 0.0173 (2) |
| C2 | 0.7199 (3) | 0.39273 (9) | 0.79124 (8) | 0.0226 (3) |
| H2A | 0.7112 | 0.4252 | 0.7453 | 0.027* |
| C3 | 0.8936 (3) | 0.41738 (9) | 0.84818 (8) | 0.0240 (3) |
| H3A | 1.0056 | 0.4666 | 0.8402 | 0.029* |
| C4 | 0.9045 (3) | 0.36954 (9) | 0.91801 (8) | 0.0223 (3) |
| H4A | 1.0230 | 0.3876 | 0.9557 | 0.027* |
| C5 | 0.7413 (3) | 0.29592 (9) | 0.93148 (7) | 0.0188 (2) |
| H5A | 0.7477 | 0.2648 | 0.9781 | 0.023* |
| C6 | 0.5668 (2) | 0.26908 (9) | 0.87415 (6) | 0.0159 (2) |
| C7 | 0.2610 (3) | 0.18779 (9) | 0.81703 (7) | 0.0171 (2) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.0085 (3) | 0.05695 (9) | 0.89446 (7) | 0.0219 (2) |
| H8A | 0.1752 | 0.0279 | 0.9053 | 0.026* |
| H8B | −0.0207 | 0.1041 | 0.9327 | 0.026* |
| C9 | −0.2085 (3) | −0.01289 (9) | 0.89821 (8) | 0.0208 (3) |
| C10 | −0.2437 (3) | −0.06360 (9) | 0.97210 (8) | 0.0197 (2) |
| C11 | −0.4423 (3) | −0.12874 (9) | 0.97723 (9) | 0.0255 (3) |
| H11A | −0.5527 | −0.1388 | 0.9355 | 0.031* |
| C12 | −0.4758 (3) | −0.17854 (10) | 1.04421 (9) | 0.0296 (3) |
| H12A | −0.6096 | −0.2215 | 1.0476 | 0.036* |
| C13 | −0.3103 (3) | −0.16447 (9) | 1.10627 (9) | 0.0271 (3) |
| H13A | −0.3309 | −0.1991 | 1.1507 | 0.032* |
| C14 | −0.1145 (3) | −0.09906 (10) | 1.10233 (8) | 0.0271 (3) |
| H14A | −0.0055 | −0.0891 | 1.1443 | 0.032* |
| C15 | −0.0816 (3) | −0.04858 (10) | 1.03552 (8) | 0.0240 (3) |
| H15A | 0.0493 | −0.0044 | 1.0329 | 0.029* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.02236 (15) | 0.02516 (15) | 0.01403 (13) | −0.00182 (12) | −0.00251 (11) | 0.00181 (11) |
| S2 | 0.02335 (15) | 0.02168 (14) | 0.01685 (13) | −0.00322 (13) | −0.00214 (12) | −0.00344 (11) |
| O1 | 0.0360 (6) | 0.0339 (5) | 0.0323 (5) | −0.0120 (5) | −0.0132 (5) | 0.0001 (4) |
| N1 | 0.0199 (5) | 0.0188 (5) | 0.0148 (5) | −0.0008 (4) | 0.0011 (4) | −0.0018 (4) |
| C1 | 0.0166 (5) | 0.0199 (5) | 0.0154 (5) | 0.0016 (4) | −0.0003 (4) | −0.0011 (4) |
| C2 | 0.0233 (6) | 0.0220 (6) | 0.0224 (6) | 0.0001 (5) | 0.0012 (5) | 0.0051 (5) |
| C3 | 0.0223 (6) | 0.0193 (6) | 0.0303 (7) | −0.0026 (5) | −0.0002 (5) | 0.0022 (5) |
| C4 | 0.0202 (6) | 0.0231 (6) | 0.0237 (6) | 0.0003 (5) | −0.0041 (5) | −0.0042 (5) |
| C5 | 0.0207 (6) | 0.0197 (6) | 0.0160 (5) | 0.0021 (5) | −0.0016 (4) | −0.0006 (4) |
| C6 | 0.0168 (5) | 0.0164 (5) | 0.0144 (5) | 0.0018 (5) | 0.0012 (4) | −0.0015 (4) |
| C7 | 0.0188 (6) | 0.0175 (5) | 0.0150 (5) | 0.0002 (4) | 0.0019 (4) | −0.0021 (4) |
| C8 | 0.0226 (6) | 0.0233 (6) | 0.0199 (5) | −0.0065 (6) | −0.0036 (5) | 0.0005 (5) |
| C9 | 0.0197 (6) | 0.0173 (6) | 0.0253 (6) | −0.0004 (5) | −0.0011 (5) | −0.0033 (5) |
| C10 | 0.0172 (6) | 0.0155 (5) | 0.0265 (6) | 0.0010 (4) | 0.0018 (5) | −0.0026 (5) |
| C11 | 0.0211 (7) | 0.0221 (6) | 0.0333 (7) | −0.0042 (5) | −0.0012 (5) | −0.0039 (5) |
| C12 | 0.0255 (7) | 0.0225 (6) | 0.0409 (8) | −0.0054 (6) | 0.0072 (6) | −0.0009 (6) |
| C13 | 0.0282 (7) | 0.0229 (6) | 0.0301 (7) | 0.0020 (6) | 0.0098 (6) | 0.0020 (5) |
| C14 | 0.0280 (7) | 0.0280 (7) | 0.0253 (6) | −0.0025 (6) | −0.0006 (5) | 0.0005 (6) |
| C15 | 0.0206 (6) | 0.0228 (6) | 0.0285 (6) | −0.0051 (5) | −0.0006 (5) | 0.0006 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.7365 (13) | C5—H5A | 0.9300 |
| S1—C7 | 1.7548 (13) | C8—C9 | 1.5080 (18) |
| S2—C7 | 1.7459 (13) | C8—H8A | 0.9700 |
| S2—C8 | 1.8022 (13) | C8—H8B | 0.9700 |
| O1—C9 | 1.2122 (16) | C9—C10 | 1.4945 (19) |
| N1—C7 | 1.2944 (16) | C10—C11 | 1.3943 (18) |
| N1—C6 | 1.3923 (17) | C10—C15 | 1.3964 (19) |

| | | | |
|---|---|---|---|
| C1—C2 | 1.3929 (18) | C11—C12 | 1.384 (2) |
| C1—C6 | 1.4073 (17) | C11—H11A | 0.9300 |
| C2—C3 | 1.3774 (19) | C12—C13 | 1.386 (2) |
| C2—H2A | 0.9300 | C12—H12A | 0.9300 |
| C3—C4 | 1.4026 (19) | C13—C14 | 1.385 (2) |
| C3—H3A | 0.9300 | C13—H13A | 0.9300 |
| C4—C5 | 1.3813 (19) | C14—C15 | 1.387 (2) |
| C4—H4A | 0.9300 | C14—H14A | 0.9300 |
| C5—C6 | 1.3934 (17) | C15—H15A | 0.9300 |

| | | | |
|---|---|---|---|
| C1—S1—C7 | 88.68 (6) | S2—C8—H8A | 109.8 |
| C7—S2—C8 | 97.66 (6) | C9—C8—H8B | 109.8 |
| C7—N1—C6 | 109.87 (11) | S2—C8—H8B | 109.8 |
| C2—C1—C6 | 121.32 (12) | H8A—C8—H8B | 108.3 |
| C2—C1—S1 | 129.51 (10) | O1—C9—C10 | 121.56 (13) |
| C6—C1—S1 | 109.17 (9) | O1—C9—C8 | 120.95 (12) |
| C3—C2—C1 | 118.08 (12) | C10—C9—C8 | 117.49 (11) |
| C3—C2—H2A | 121.0 | C11—C10—C15 | 119.22 (13) |
| C1—C2—H2A | 121.0 | C11—C10—C9 | 118.78 (12) |
| C2—C3—C4 | 121.17 (13) | C15—C10—C9 | 121.99 (12) |
| C2—C3—H3A | 119.4 | C12—C11—C10 | 120.20 (14) |
| C4—C3—H3A | 119.4 | C12—C11—H11A | 119.9 |
| C5—C4—C3 | 120.77 (12) | C10—C11—H11A | 119.9 |
| C5—C4—H4A | 119.6 | C11—C12—C13 | 120.13 (13) |
| C3—C4—H4A | 119.6 | C11—C12—H12A | 119.9 |
| C4—C5—C6 | 118.93 (12) | C13—C12—H12A | 119.9 |
| C4—C5—H5A | 120.5 | C14—C13—C12 | 120.25 (13) |
| C6—C5—H5A | 120.5 | C14—C13—H13A | 119.9 |
| N1—C6—C5 | 124.71 (11) | C12—C13—H13A | 119.9 |
| N1—C6—C1 | 115.57 (10) | C13—C14—C15 | 119.76 (14) |
| C5—C6—C1 | 119.71 (12) | C13—C14—H14A | 120.1 |
| N1—C7—S2 | 125.63 (10) | C15—C14—H14A | 120.1 |
| N1—C7—S1 | 116.71 (10) | C14—C15—C10 | 120.42 (13) |
| S2—C7—S1 | 117.63 (7) | C14—C15—H15A | 119.8 |
| C9—C8—S2 | 109.28 (9) | C10—C15—H15A | 119.8 |
| C9—C8—H8A | 109.8 | | |

| | | | |
|---|---|---|---|
| C7—S1—C1—C2 | 179.53 (13) | C8—S2—C7—S1 | −172.57 (8) |
| C7—S1—C1—C6 | 0.04 (9) | C1—S1—C7—N1 | 0.00 (11) |
| C6—C1—C2—C3 | 0.86 (19) | C1—S1—C7—S2 | 177.93 (8) |
| S1—C1—C2—C3 | −178.59 (11) | C7—S2—C8—C9 | 175.74 (9) |
| C1—C2—C3—C4 | −1.0 (2) | S2—C8—C9—O1 | −0.42 (16) |
| C2—C3—C4—C5 | 0.2 (2) | S2—C8—C9—C10 | 179.05 (10) |
| C3—C4—C5—C6 | 0.7 (2) | O1—C9—C10—C11 | −0.4 (2) |
| C7—N1—C6—C5 | −179.59 (12) | C8—C9—C10—C11 | −179.87 (12) |
| C7—N1—C6—C1 | 0.07 (15) | O1—C9—C10—C15 | 178.67 (13) |
| C4—C5—C6—N1 | 178.80 (12) | C8—C9—C10—C15 | −0.79 (18) |
| C4—C5—C6—C1 | −0.84 (19) | C15—C10—C11—C12 | −0.7 (2) |

| | | | |
|---|---|---|---|
| C2—C1—C6—N1 | −179.62 (11) | C9—C10—C11—C12 | 178.35 (13) |
| S1—C1—C6—N1 | −0.07 (13) | C10—C11—C12—C13 | −0.6 (2) |
| C2—C1—C6—C5 | 0.06 (19) | C11—C12—C13—C14 | 1.5 (2) |
| S1—C1—C6—C5 | 179.61 (10) | C12—C13—C14—C15 | −1.0 (2) |
| C6—N1—C7—S2 | −177.78 (9) | C13—C14—C15—C10 | −0.3 (2) |
| C6—N1—C7—S1 | −0.04 (14) | C11—C10—C15—C14 | 1.2 (2) |
| C8—S2—C7—N1 | 5.15 (13) | C9—C10—C15—C14 | −177.84 (13) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2*A*···O1$^{i}$ | 0.93 | 2.51 | 3.2299 (17) | 135 |

Symmetry code: (i) −*x*, *y*+1/2, −*z*+3/2.