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# (5*Z*)-5-(2-Hydroxybenzylidene)-3-phenyl-2-thioxo-1,3-thiazolidin-4-one

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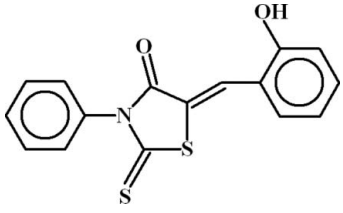
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.102; data-to-parameter ratio = 18.2.

In the title compound, $C_{16}H_{11}NO_2S_2$, the dihedral angles between the heterocyclic ring and the phenyl and anilinic benzene rings are 9.68 (13) and 79.26 (6)°, respectively, and an intramolecular C—H···S interaction occurs. In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds occur, leading to $R_2^2(10)$ loops, and C—H···O and weak C—H···$\pi$ interactions further consolidate the packing.

## Related literature

For related structures, see: Linden *et al.* (1999); Shahwar *et al.* (2009*a*, 2009*b*). For graph-set theory, see: Bernstein *et al.* (1995).




## Experimental

### Crystal data

$C_{16}H_{11}NO_2S_2$
$M_r$ = 313.40
Monoclinic, $P2_1/n$
$a$ = 11.6553 (7) Å
$b$ = 7.3424 (4) Å
$c$ = 16.8256 (10) Å
$\beta$ = 95.131 (2)°
$V$ = 1434.13 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.37 mm$^{-1}$
$T$ = 296 K
0.26 × 0.18 × 0.17 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.924, $T_{max}$ = 0.937
15580 measured reflections
3481 independent reflections
2194 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.102
$S$ = 1.01
3481 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C16—H16···S1 | 0.93 | 2.50 | 3.213 (2) | 133 |
| O2—H2$A$···O1$^{i}$ | 0.82 | 1.97 | 2.767 (2) | 163 |
| C10—H10···O2$^{i}$ | 0.93 | 2.49 | 3.375 (3) | 160 |
| C2—H2···Cg$B^{ii}$ | 0.93 | 2.91 | 3.774 (2) | 155 |
| C14—H14···Cg$B^{iii}$ | 0.93 | 2.91 | 3.515 (2) | 124 |

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$. *CgB* is the centroid of the C1–C6 ring.

Data collection: *APEX2* (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: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5180).

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# supporting information

*Acta Cryst.* (2009). E**65**, o2903 [https://doi.org/10.1107/S1600536809044286]

## (5*Z*)-5-(2-Hydroxybenzylidene)-3-phenyl-2-thioxo-1,3-thiazolidin-4-one

**Durre Shahwar, M. Nawaz Tahir, Muhammad Asam Raza and Bushra Iqbal**

### S1. Comment

We have recently reported the crystal structure of (II) (5*Z*)-5-(2-Hydroxybenzylidene)-2-thioxo-1,3-thiazolidin-4- one methanol hemisolvate (Shahwar *et al.*, 2009*a*) and (III) (5*E*)-5-(4-Hydroxy-3-methoxybenzylidene)-2-thioxo-1,3-thiazolidin- 4-one methanol monosolvate (Shahwar *et al.*, 2009*b*) which contain the rhodanine. In continuation of synthesizing various derivatives of rhodanine, the title compound (I, Fig. 1), is being reported. The crystal structure of (IV) 3-Phenyl-5-(phenylmethylidene)-2-thioxo-1,3-thiazolidin-4-one (Linden *et al.*, 1999) has also been published. Title compound (I) differs from (IV) due to attachement of hydroxy group with benzylidene.

In (I) the heterocyclic ring A (N1/C7/S1/C8/C9), two benzene rings B (C1—C6) and C (C11–C16) are planar with maximum r. m. s. deviations of 0.0145, 0.0038 and 0.0070 Å respectively, from the respective mean square planes. The dihedral angles between A/B, A/C and B/C are 79.26 (6), 9.68 (13) and 69.62 (6)°, respectively. The intramolecular H-bondings of C—H···S (Table 1, Fig. 1) form twisted S(6) ring motif (Bernstein *et al.*, 1995). The molecules of (I) are stabilized in the form of dimers due to intermolecular H-bondings (Table 1, Fig. 2) froming $R_2^2(7)$ and $R_2^2(10)$ ring motifs. The C–H···$\pi$ interactions (Table 1) also play role in stabilizing the molecules.

### S2. Experimental

3-Phenyl-2-thioxo-1,3-thiazolidin-4-one (0.419 g, 0.2 mol), 2-Hydroxybenzaldehyde (0.244 g, 0.2 mol) and $K_2CO_3$ (0.553 g, 0.4 mol) were dissolved in 10 ml distilled water at room temperature. The stirring was continued for 24 h and reaction was monitored by TLC. The precipitates were formed during neutalization of the reaction mixture with 5% HCl. The precipitates were filtered off and washed with saturated solution of NaCl. The crude material obtained was recrystalized in ethyl acetate to affoard orange yellow prisms of (I).

### S3. Refinement

The H-atoms were positioned geometrically (O–H = 0.82 Å, C–H = 0.93 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(O).

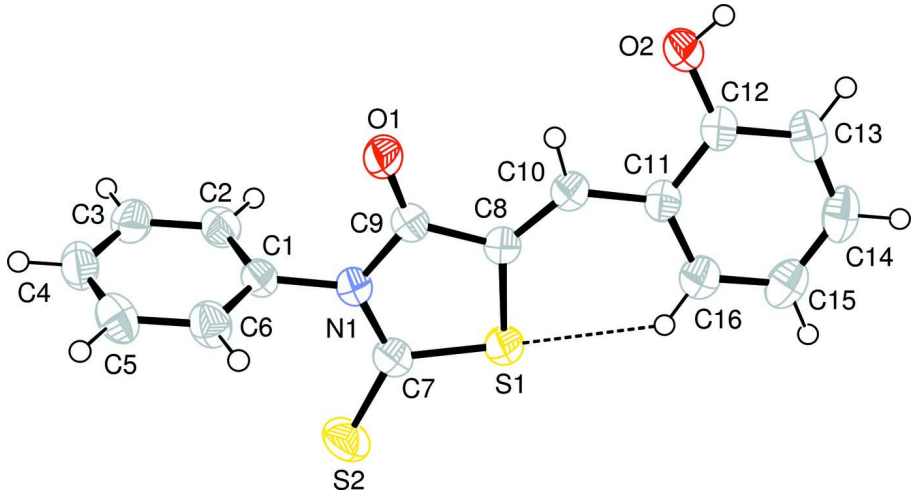


**Figure 1**

View of (I) with displacement ellipsoids drawn at the 50% probability level. The dotted line represents the intramolecular H-bond.

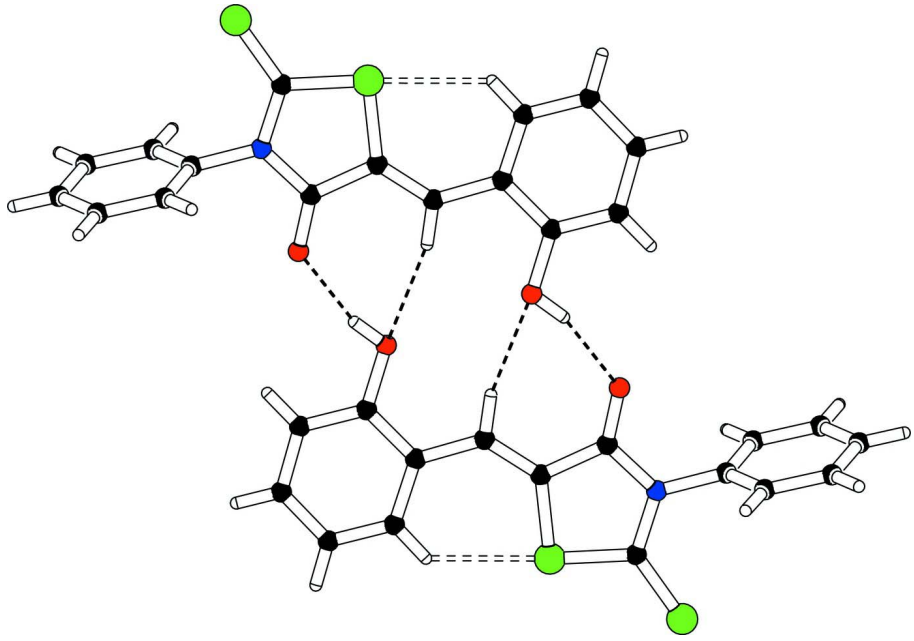

**Figure 2**

The partial packing of (I), which shows that molecules form inversion dimers.

**(5*Z*)-5-(2-Hydroxybenzylidene)-3-phenyl-2-thioxo-1,3-thiazolidin-4-one**

*Crystal data*

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$a = 11.6553\ (7)$ Å
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$c = 16.8256\ (10)$ Å
$\beta = 95.131\ (2)°$
$V = 1434.13\ (14)$ Å$^3$
$Z = 4$
$F(000) = 648$
$D_x = 1.452$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3481 reflections

$\theta$ = 2.0–28.0°
$\mu$ = 0.37 mm$^{-1}$
$T$ = 296 K

Prisms, orange yellow
0.26 × 0.18 × 0.17 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.40 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.924, $T_{max}$ = 0.937

15580 measured reflections
3481 independent reflections
2194 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 28.0°, $\theta_{min}$ = 2.0°
$h$ = −15→14
$k$ = −9→9
$l$ = −22→22

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.102
$S$ = 1.01
3481 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.326P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.16936 (5) | 0.50419 (7) | 0.48587 (3) | 0.0463 (2) |
| S2 | 0.12725 (6) | 0.16709 (8) | 0.57270 (4) | 0.0591 (2) |
| O1 | 0.45774 (15) | 0.5967 (2) | 0.60654 (9) | 0.0572 (6) |
| O2 | 0.40155 (14) | 1.1358 (2) | 0.44795 (9) | 0.0515 (6) |
| N1 | 0.30920 (15) | 0.3922 (2) | 0.60195 (9) | 0.0376 (6) |
| C1 | 0.35642 (18) | 0.2866 (3) | 0.66982 (12) | 0.0370 (7) |
| C2 | 0.3410 (2) | 0.3461 (3) | 0.74551 (12) | 0.0432 (7) |
| C3 | 0.3835 (2) | 0.2416 (3) | 0.81002 (12) | 0.0477 (8) |
| C4 | 0.4398 (2) | 0.0815 (3) | 0.79786 (14) | 0.0497 (8) |
| C5 | 0.4550 (2) | 0.0235 (3) | 0.72188 (14) | 0.0524 (9) |
| C6 | 0.4139 (2) | 0.1273 (3) | 0.65678 (13) | 0.0466 (8) |
| C7 | 0.20684 (19) | 0.3439 (3) | 0.55947 (12) | 0.0399 (7) |
| C8 | 0.29274 (19) | 0.6347 (3) | 0.51013 (11) | 0.0385 (7) |
| C9 | 0.3643 (2) | 0.5470 (3) | 0.57636 (12) | 0.0401 (7) |

| | | | | |
|---|---|---|---|---|
| C10 | 0.32304 (19) | 0.7938 (3) | 0.47846 (12) | 0.0418 (7) |
| C11 | 0.26629 (19) | 0.9014 (3) | 0.41462 (11) | 0.0379 (7) |
| C12 | 0.31041 (19) | 1.0743 (3) | 0.39934 (12) | 0.0389 (7) |
| C13 | 0.2611 (2) | 1.1796 (3) | 0.33719 (13) | 0.0494 (8) |
| C14 | 0.1673 (2) | 1.1153 (3) | 0.28976 (13) | 0.0540 (9) |
| C15 | 0.1207 (2) | 0.9486 (3) | 0.30463 (13) | 0.0533 (9) |
| C16 | 0.1702 (2) | 0.8438 (3) | 0.36550 (13) | 0.0478 (8) |
| H2 | 0.30268 | 0.45483 | 0.75331 | 0.0518* |
| H2A | 0.43058 | 1.22336 | 0.42710 | 0.0772* |
| H3 | 0.37382 | 0.28003 | 0.86166 | 0.0572* |
| H4 | 0.46807 | 0.01166 | 0.84139 | 0.0596* |
| H5 | 0.49284 | −0.08572 | 0.71418 | 0.0629* |
| H6 | 0.42501 | 0.08995 | 0.60520 | 0.0559* |
| H10 | 0.39181 | 0.84263 | 0.50141 | 0.0502* |
| H13 | 0.29121 | 1.29390 | 0.32743 | 0.0593* |
| H14 | 0.13538 | 1.18544 | 0.24737 | 0.0648* |
| H15 | 0.05592 | 0.90715 | 0.27356 | 0.0640* |
| H16 | 0.13881 | 0.72999 | 0.37452 | 0.0574* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0458 (4) | 0.0443 (3) | 0.0466 (3) | −0.0085 (3) | −0.0083 (2) | 0.0067 (2) |
| S2 | 0.0556 (4) | 0.0454 (3) | 0.0756 (4) | −0.0154 (3) | 0.0014 (3) | 0.0099 (3) |
| O1 | 0.0538 (11) | 0.0551 (10) | 0.0582 (10) | −0.0197 (8) | −0.0194 (8) | 0.0209 (8) |
| O2 | 0.0534 (11) | 0.0476 (9) | 0.0518 (9) | −0.0149 (8) | −0.0042 (8) | 0.0148 (7) |
| N1 | 0.0414 (11) | 0.0340 (9) | 0.0369 (9) | −0.0023 (8) | 0.0001 (8) | 0.0047 (7) |
| C1 | 0.0387 (13) | 0.0322 (10) | 0.0397 (11) | −0.0023 (9) | 0.0020 (9) | 0.0042 (8) |
| C2 | 0.0475 (14) | 0.0371 (11) | 0.0449 (12) | 0.0020 (10) | 0.0036 (10) | 0.0007 (9) |
| C3 | 0.0533 (16) | 0.0514 (13) | 0.0380 (12) | −0.0027 (12) | 0.0027 (10) | 0.0026 (10) |
| C4 | 0.0480 (15) | 0.0486 (13) | 0.0514 (14) | −0.0004 (11) | −0.0012 (11) | 0.0169 (11) |
| C5 | 0.0556 (17) | 0.0388 (12) | 0.0631 (15) | 0.0100 (11) | 0.0071 (12) | 0.0076 (10) |
| C6 | 0.0573 (16) | 0.0412 (12) | 0.0424 (12) | 0.0060 (10) | 0.0100 (11) | 0.0015 (9) |
| C7 | 0.0418 (14) | 0.0364 (11) | 0.0418 (11) | −0.0014 (10) | 0.0053 (9) | 0.0003 (9) |
| C8 | 0.0427 (13) | 0.0362 (11) | 0.0357 (11) | −0.0038 (9) | −0.0014 (9) | 0.0027 (8) |
| C9 | 0.0463 (15) | 0.0355 (11) | 0.0378 (11) | −0.0051 (9) | 0.0004 (10) | 0.0036 (8) |
| C10 | 0.0428 (14) | 0.0422 (12) | 0.0391 (11) | −0.0053 (10) | −0.0038 (9) | 0.0042 (9) |
| C11 | 0.0391 (13) | 0.0406 (11) | 0.0337 (11) | 0.0012 (10) | 0.0025 (9) | 0.0042 (8) |
| C12 | 0.0390 (13) | 0.0428 (11) | 0.0350 (11) | 0.0039 (10) | 0.0040 (9) | 0.0054 (9) |
| C13 | 0.0561 (16) | 0.0453 (12) | 0.0478 (13) | 0.0090 (11) | 0.0097 (12) | 0.0138 (10) |
| C14 | 0.0571 (17) | 0.0631 (16) | 0.0413 (13) | 0.0211 (13) | 0.0025 (12) | 0.0134 (11) |
| C15 | 0.0471 (16) | 0.0672 (16) | 0.0438 (13) | 0.0075 (12) | −0.0066 (11) | 0.0018 (11) |
| C16 | 0.0488 (15) | 0.0485 (13) | 0.0451 (12) | −0.0022 (11) | −0.0019 (10) | 0.0041 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C7 | 1.736 (2) | C10—C11 | 1.445 (3) |
| S1—C8 | 1.746 (2) | C11—C16 | 1.397 (3) |

| | | | |
|---|---|---|---|
| S2—C7 | 1.623 (2) | C11—C12 | 1.402 (3) |
| O1—C9 | 1.216 (3) | C12—C13 | 1.384 (3) |
| O2—C12 | 1.359 (3) | C13—C14 | 1.378 (3) |
| O2—H2A | 0.8200 | C14—C15 | 1.371 (3) |
| N1—C7 | 1.381 (3) | C15—C16 | 1.367 (3) |
| N1—C9 | 1.393 (3) | C2—H2 | 0.9300 |
| N1—C1 | 1.448 (3) | C3—H3 | 0.9300 |
| C1—C6 | 1.375 (3) | C4—H4 | 0.9300 |
| C1—C2 | 1.373 (3) | C5—H5 | 0.9300 |
| C2—C3 | 1.384 (3) | C6—H6 | 0.9300 |
| C3—C4 | 1.371 (3) | C10—H10 | 0.9300 |
| C4—C5 | 1.374 (3) | C13—H13 | 0.9300 |
| C5—C6 | 1.384 (3) | C14—H14 | 0.9300 |
| C8—C9 | 1.479 (3) | C15—H15 | 0.9300 |
| C8—C10 | 1.344 (3) | C16—H16 | 0.9300 |

| | | | |
|---|---|---|---|
| C7—S1—C8 | 93.20 (10) | C11—C12—C13 | 120.7 (2) |
| C12—O2—H2A | 109.00 | O2—C12—C11 | 118.06 (18) |
| C1—N1—C9 | 121.85 (17) | C12—C13—C14 | 120.1 (2) |
| C7—N1—C9 | 116.78 (17) | C13—C14—C15 | 120.5 (2) |
| C1—N1—C7 | 121.37 (16) | C14—C15—C16 | 119.5 (2) |
| N1—C1—C6 | 119.07 (18) | C11—C16—C15 | 122.4 (2) |
| C2—C1—C6 | 121.6 (2) | C1—C2—H2 | 121.00 |
| N1—C1—C2 | 119.28 (19) | C3—C2—H2 | 121.00 |
| C1—C2—C3 | 118.9 (2) | C2—C3—H3 | 120.00 |
| C2—C3—C4 | 120.1 (2) | C4—C3—H3 | 120.00 |
| C3—C4—C5 | 120.5 (2) | C3—C4—H4 | 120.00 |
| C4—C5—C6 | 120.1 (2) | C5—C4—H4 | 120.00 |
| C1—C6—C5 | 118.8 (2) | C4—C5—H5 | 120.00 |
| S1—C7—S2 | 122.00 (13) | C6—C5—H5 | 120.00 |
| S1—C7—N1 | 110.23 (15) | C1—C6—H6 | 121.00 |
| S2—C7—N1 | 127.77 (16) | C5—C6—H6 | 121.00 |
| S1—C8—C9 | 109.54 (15) | C8—C10—H10 | 115.00 |
| S1—C8—C10 | 128.64 (17) | C11—C10—H10 | 115.00 |
| C9—C8—C10 | 121.8 (2) | C12—C13—H13 | 120.00 |
| O1—C9—C8 | 127.4 (2) | C14—C13—H13 | 120.00 |
| N1—C9—C8 | 110.11 (18) | C13—C14—H14 | 120.00 |
| O1—C9—N1 | 122.45 (19) | C15—C14—H14 | 120.00 |
| C8—C10—C11 | 130.6 (2) | C14—C15—H15 | 120.00 |
| C10—C11—C16 | 124.3 (2) | C16—C15—H15 | 120.00 |
| C12—C11—C16 | 116.97 (19) | C11—C16—H16 | 119.00 |
| C10—C11—C12 | 118.71 (19) | C15—C16—H16 | 119.00 |
| O2—C12—C13 | 121.3 (2) | | |

| | | | |
|---|---|---|---|
| C8—S1—C7—S2 | −179.12 (15) | C3—C4—C5—C6 | 0.3 (4) |
| C8—S1—C7—N1 | 1.29 (16) | C4—C5—C6—C1 | −1.1 (3) |
| C7—S1—C8—C9 | 0.95 (16) | S1—C8—C9—O1 | 177.26 (19) |
| C7—S1—C8—C10 | −177.2 (2) | S1—C8—C9—N1 | −2.9 (2) |

| | | | |
|---|---|---|---|
| C7—N1—C1—C2 | −99.9 (2) | C10—C8—C9—O1 | −4.5 (4) |
| C7—N1—C1—C6 | 78.9 (3) | C10—C8—C9—N1 | 175.33 (19) |
| C9—N1—C1—C2 | 80.0 (3) | S1—C8—C10—C11 | −1.9 (4) |
| C9—N1—C1—C6 | −101.2 (2) | C9—C8—C10—C11 | −179.8 (2) |
| C1—N1—C7—S1 | 176.46 (14) | C8—C10—C11—C12 | 172.8 (2) |
| C1—N1—C7—S2 | −3.1 (3) | C8—C10—C11—C16 | −8.2 (4) |
| C9—N1—C7—S1 | −3.5 (2) | C10—C11—C12—O2 | −3.0 (3) |
| C9—N1—C7—S2 | 176.98 (17) | C10—C11—C12—C13 | 177.9 (2) |
| C1—N1—C9—O1 | 4.1 (3) | C16—C11—C12—O2 | 177.90 (19) |
| C1—N1—C9—C8 | −175.75 (17) | C16—C11—C12—C13 | −1.2 (3) |
| C7—N1—C9—O1 | −176.0 (2) | C10—C11—C16—C15 | −178.6 (2) |
| C7—N1—C9—C8 | 4.2 (2) | C12—C11—C16—C15 | 0.5 (3) |
| N1—C1—C2—C3 | 178.1 (2) | O2—C12—C13—C14 | −178.7 (2) |
| C6—C1—C2—C3 | −0.7 (3) | C11—C12—C13—C14 | 0.3 (3) |
| N1—C1—C6—C5 | −177.6 (2) | C12—C13—C14—C15 | 1.3 (3) |
| C2—C1—C6—C5 | 1.3 (3) | C13—C14—C15—C16 | −2.0 (3) |
| C1—C2—C3—C4 | −0.1 (3) | C14—C15—C16—C11 | 1.1 (3) |
| C2—C3—C4—C5 | 0.2 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16···S1 | 0.93 | 2.50 | 3.213 (2) | 133 |
| O2—H2*A*···O1$^{i}$ | 0.82 | 1.97 | 2.767 (2) | 163 |
| C10—H10···O2$^{i}$ | 0.93 | 2.49 | 3.375 (3) | 160 |
| C2—H2···CgB$^{ii}$ | 0.93 | 2.91 | 3.774 (2) | 155 |
| C14—H14···CgB$^{iii}$ | 0.93 | 2.91 | 3.515 (2) | 124 |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) *x*−1/2, −*y*+3/2, *z*−1/2.