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N-[(*E,Z*)-1,3-Diphenylprop-2-enylidene]-*N'*-(1,3-dithiolan-2-ylidene)hydrazine

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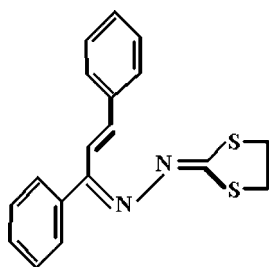
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.046; wR factor = 0.118; data-to-parameter ratio = 16.2.

Molecules of the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{S}_2$, exist as the (*2E*, *1'Z*)-isomer. The 1,3-dithiolane ring has an envelope conformation; the atoms of the C—C bond are disordered over two positions with occupancies of 0.47 (7) and 0.53 (7). The structure exhibits intermolecular C—H \cdots S and C—H \cdots π (arene) hydrogen bonds.

Related literature

For related literature, see: Beghidja *et al.* (2006); Cremer & Pople (1975); Gou *et al.* (2004); Liu *et al.* (2001, 2003, 2007, 2008); Wang *et al.* (1994); Xu *et al.* (2005); Yang *et al.* (2007); Yarishkin *et al.* (2008); Zhai *et al.* (1999).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_2\text{S}_2$
 $M_r = 324.47$
 Orthorhombic, $Pna2_1$
 $a = 30.9008$ (9) Å
 $b = 5.7352$ (2) Å
 $c = 9.1499$ (3) Å

$V = 1621.57$ (9) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.33$ mm⁻¹
 $T = 296$ (2) K
 $0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART 1000 CCD
 diffractometer

Absorption correction: multi-scan
 (SADABS; Bruker, 2007)
 $T_{\min} = 0.909$, $T_{\max} = 0.938$

7320 measured reflections
 3339 independent reflections

2833 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.117$
 $S = 1.00$
 3339 reflections
 206 parameters
 7 restraints

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.47$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³
 Absolute structure: Flack (1983),
 1186 Friedel pairs
 Flack parameter: -0.03 (9)

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C17}-\text{H17B}\cdots\text{Cg}^{\text{i}}$ | 0.97 | 2.94 | 3.842 (9) | 156 |
| $\text{C18}'-\text{H18A}\cdots\text{S1}^{\text{ii}}$ | 0.97 | 2.69 | 3.439 (6) | 135 |
| $\text{C18}'-\text{H18B}\cdots\text{S1}^{\text{i}}$ | 0.97 | 2.86 | 3.628 (7) | 137 |

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$. Cg is the centroid of atoms C10–C15.

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: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2242).

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supporting information

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***N*-[(*E,Z*)-1,3-Diphenylprop-2-enylidene]-*N'*-(1,3-dithiolan-2-ylidene)hydrazine**

Jian-Feng Liu, Xiao-Lan Liu and Yong-Hong Liu

S1. Comment

The Schiff bases and carbonyl derivatives of 2-hydrazono-1, 3-dithiolane have been abstracted for their coordination chemistry and biological activity (Beghidja *et al.*, 2006; Wang *et al.*, 1994, Gou *et al.*, 2004; Xu *et al.*, 2005). Chalcone and its derivatives, as a natural products, have shown strong antibacterial, antifungal, antitumor and anti-inflammatory properties, especially antileishmanial, antimalarial and antimalarial (Zhai *et al.*, 1999; Liu *et al.*, 2001, 2003). Some chalcones demonstrated the ability to block voltage-dependent potassium channels (Yarishkin *et al.*, 2008). As ongoing research (Liu *et al.*, 2008, Yang *et al.*, 2007), we report herein the synthesis and structure of the title compound *via* the condensation reaction of the simple chalcone, (*E*)-1,3-diphenyl-propenone, and 2-hydrazono-1, 3-dithiolane.

The molecule of the title compound exists as the most stable configuration of (*2E, 1'Z*)-isomer (Fig.1). In the molecule the atoms of C16, N2, N1, C9, C8, C7 and two phenyl rings form a large conjugated system, but only the atoms of S1, S2, C16, N2, N1, C9 and C8 are coplanar, and C7, C6 and C10 are deviate by 0.22, 0.24, 0.11 (2) Å from the plane, respectively. The dihedral angles between the plane to phenyl ring (C10 ~ C15) plane and (C1~C6) plane are 63.45 (2)° and 43.30 (18)°, respectively. The two phenyl ring planes are almost vertical (the dihedral angle between them is 84.16°) (Fig. 1, Table 2).

In the ring of 1, 3-dithiolane of the molecule, the atoms of C17 and C18 are disordered over two positions with relative occupancies of 0.43 (7):0.57 (7) for the minor and major components. The rings at the two positions are also in the envelope (Cremer *et al.*, 1975) form, and atoms C18 and C18' respectively deviate by - 0.367 (3) Å and 0.402 (2) Å from the plane defined by S1, C16 and S2, just like that in (*3E*)-3-(1, 3-dithiolan-2-ylidenehydrazono)buton (Liu *et al.*, 2007).

In its packing structure, the molecules are linked into a three-dimensional framework by C–H···S and C–H··· π (arene) intermolecular hydrogen bonds in the major components (Fig. 2 and 3, Table 2).

S2. Experimental

The title compound was prepared from (*E*)-1, 3-diphenyl-propenone and 2-hydrazono-1, 3-dithiolane in the equimolar ratio in 95% EtOH. The resulting yellow solid was recrystallized from CH₂Cl₂–EtOH to give crystals of suitable for single-crystal X-ray diffraction (yield 88%, m.p. 440–442 K). Analysis calculated for C₁₈H₁₆N₂S₂: C, 66.63; H, 4.97; N, 8.63%; found: C, 66.36; H, 4.81; N, 8.28. ¹H NMR (600 MHz, CDCl₃, δ , p.p.m.): 7.879(d, J=16.47 Hz, 1H, CH=C), 6.891(d, J=16.54 Hz, 1H, CH=C), 7.324~7.677(m, 10H, 2C₆H₅), 3.521(m, 2H, CH₂), 3.460(m, 2H, CH₂).

S3. Refinement

The C17 and C18 atoms were refined as disordered with refined occupancy of 57.3 (7) % for the major component. The anisotropic displacement parameters of C17, C17', C18 and C18' were constrained to be equal. After their location in a difference map, all H atoms were fixed geometrically at ideal positions and allowed to ride on the parent C atoms, with C—H distances of 0.93 (aromatic and ethylenic CH) or 0.97 Å (methene), and with $U_{iso}(H)$ values of 1.2 $U_{eq}(C)$.

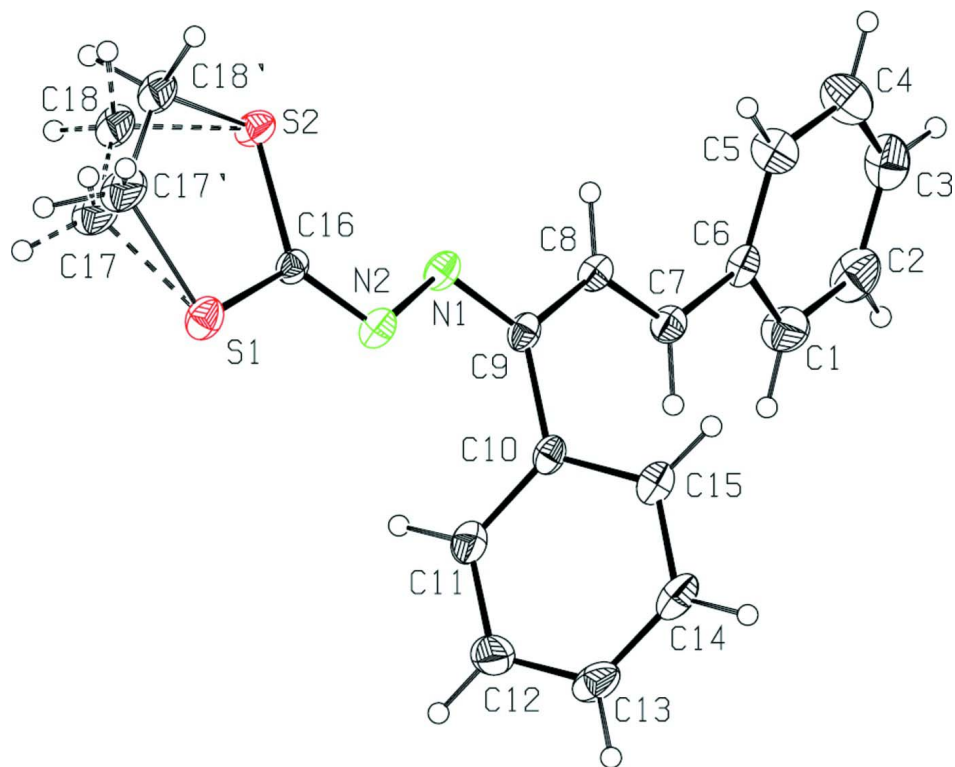
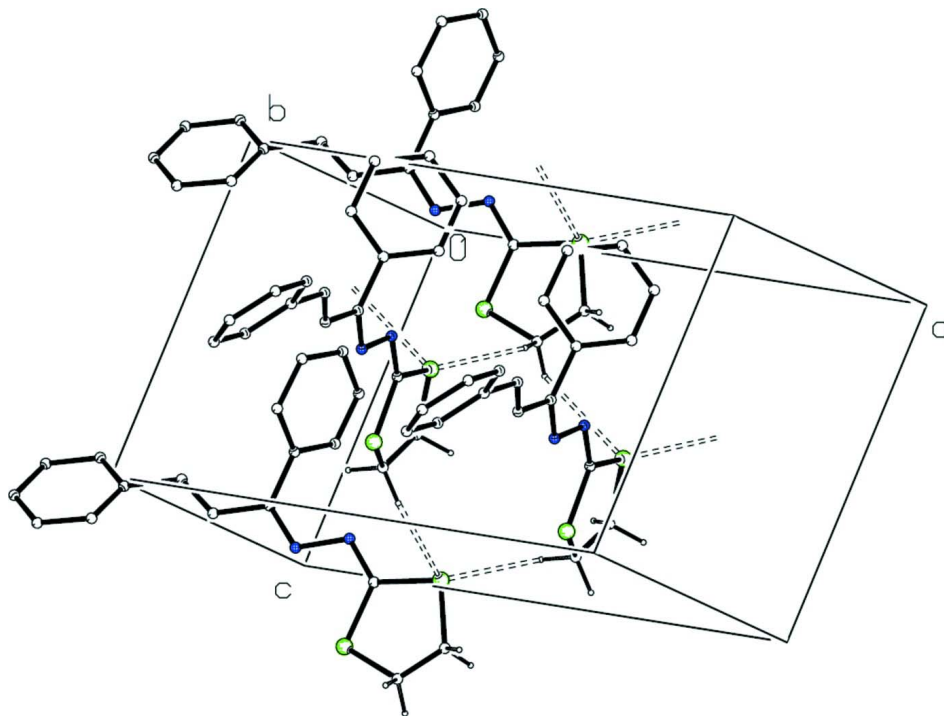
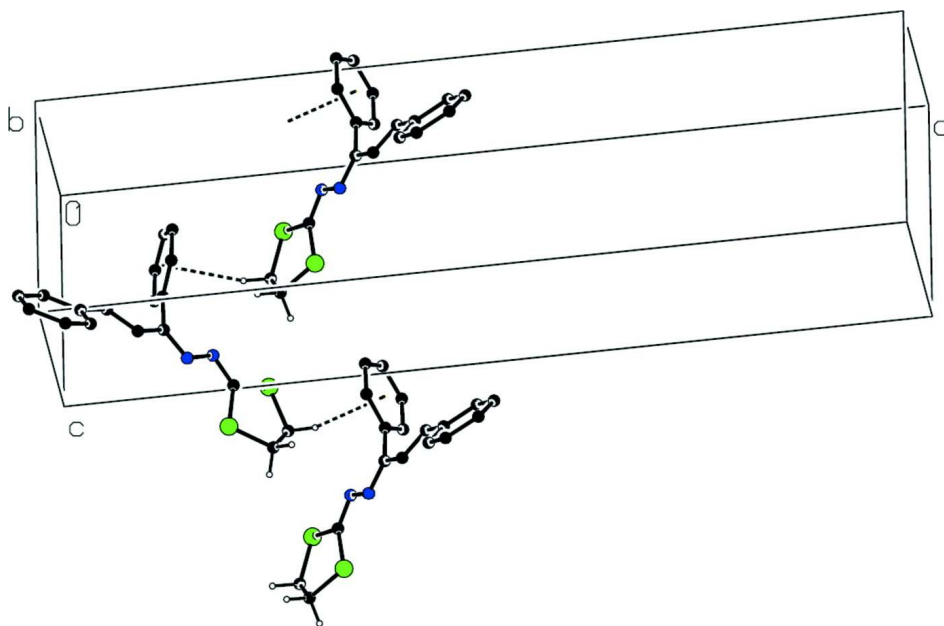


Figure 1

The molecular structure of the title compound, showing 30% probability ellipsoids. Open bonds show the minor disorder component.

**Figure 2**

Part of the crystal structure, showing C–H...S inter-molecular hydrogen bonds as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted.

**Figure 3**

Part of the crystal structure, showing C–H... π as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted.

N*-[*(E,Z)*-1,3-Diphenylprop-2-enylidene]- *N'*-(1,3-dithiolan-2-ylidene)-hydrazineCrystal data*C₁₈H₁₆N₂S₂ $M_r = 324.47$ Orthorhombic, *Pna*2₁

Hall symbol: P 2c -2n

 $a = 30.9008$ (9) Å $b = 5.7352$ (2) Å $c = 9.1499$ (3) Å $V = 1621.57$ (9) Å³ $Z = 4$ $F(000) = 680$ $D_x = 1.329$ Mg m⁻³

Melting point: 442 K

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 2883 reflections

 $\theta = 2.6$ – 28.1° $\mu = 0.33$ mm⁻¹ $T = 296$ K

Block, yellow

0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1000 CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2007)

 $T_{\min} = 0.909$, $T_{\max} = 0.938$

7320 measured reflections

3339 independent reflections

2833 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.055$ $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 2.6^\circ$ $h = -41 \rightarrow 39$ $k = -4 \rightarrow 7$ $l = -12 \rightarrow 11$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.117$ $S = 1.00$

3339 reflections

206 parameters

7 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

 $w = 1/[\sigma^2(F_o^2) + (0.0727P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.003$ $\Delta\rho_{\max} = 0.47$ e Å⁻³ $\Delta\rho_{\min} = -0.34$ e Å⁻³

Absolute structure: Flack (1983), 1186 Friedel

pairs

Absolute structure parameter: -0.03 (9)*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 (Å²)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|----|---------------|------------|------------|----------------------------------|-----------|
| C1 | 0.00882 (11) | 1.1023 (6) | 0.9703 (5) | 0.0507 (8) | |
| H1 | -0.0016 | 1.0304 | 0.8863 | 0.061* | |
| C2 | -0.01559 (12) | 1.2737 (7) | 1.0391 (5) | 0.0569 (10) | |

| | | | | | |
|------|---------------|---------------|-------------|--------------|-----------|
| H2 | -0.0428 | 1.3112 | 1.0024 | 0.068* | |
| C3 | -0.00045 (12) | 1.3879 (6) | 1.1592 (4) | 0.0526 (9) | |
| H3 | -0.0168 | 1.5053 | 1.2025 | 0.063* | |
| C4 | 0.03941 (11) | 1.3275 (7) | 1.2162 (5) | 0.0547 (9) | |
| H4 | 0.0500 | 1.4039 | 1.2985 | 0.066* | |
| C5 | 0.06363 (10) | 1.1535 (6) | 1.1509 (4) | 0.0423 (7) | |
| H5 | 0.0903 | 1.1133 | 1.1908 | 0.051* | |
| C6 | 0.04918 (9) | 1.0381 (5) | 1.0281 (3) | 0.0321 (6) | |
| C7 | 0.07453 (9) | 0.8558 (5) | 0.9542 (3) | 0.0318 (6) | |
| H7 | 0.0679 | 0.8263 | 0.8568 | 0.038* | |
| C8 | 0.10609 (9) | 0.7288 (5) | 1.0139 (3) | 0.0302 (6) | |
| H8 | 0.1126 | 0.7561 | 1.1117 | 0.036* | |
| C9 | 0.13112 (8) | 0.5516 (5) | 0.9387 (3) | 0.0288 (6) | |
| C10 | 0.13030 (9) | 0.5395 (5) | 0.7762 (3) | 0.0287 (6) | |
| C11 | 0.11505 (11) | 0.3437 (6) | 0.7030 (4) | 0.0400 (7) | |
| H11 | 0.1039 | 0.2189 | 0.7559 | 0.048* | |
| C12 | 0.11627 (13) | 0.3328 (7) | 0.5522 (4) | 0.0485 (9) | |
| H12 | 0.1059 | 0.2011 | 0.5044 | 0.058* | |
| C13 | 0.13278 (10) | 0.5157 (6) | 0.4720 (4) | 0.0457 (8) | |
| H13 | 0.1341 | 0.5062 | 0.3706 | 0.055* | |
| C14 | 0.14728 (10) | 0.7122 (6) | 0.5424 (4) | 0.0424 (8) | |
| H14 | 0.1581 | 0.8365 | 0.4883 | 0.051* | |
| C15 | 0.14592 (9) | 0.7269 (6) | 0.6941 (3) | 0.0352 (7) | |
| H15 | 0.1554 | 0.8615 | 0.7408 | 0.042* | |
| C16 | 0.19817 (8) | 0.1107 (5) | 1.0334 (3) | 0.0267 (6) | |
| C17 | 0.2416 (6) | -0.261 (2) | 1.1233 (8) | 0.061 (3) | 0.427 (7) |
| H17C | 0.2319 | -0.4193 | 1.1064 | 0.073* | 0.427 (7) |
| H17D | 0.2724 | -0.2661 | 1.1438 | 0.073* | 0.427 (7) |
| C18 | 0.2200 (3) | -0.1717 (16) | 1.2466 (9) | 0.0409 (13) | 0.427 (7) |
| H18C | 0.2410 | -0.1558 | 1.3248 | 0.049* | 0.427 (7) |
| H18D | 0.1989 | -0.2864 | 1.2778 | 0.049* | 0.427 (7) |
| C17' | 0.2517 (3) | -0.1970 (15) | 1.1350 (5) | 0.061 (3) | 0.573 (7) |
| H17A | 0.2432 | -0.3591 | 1.1449 | 0.073* | 0.573 (7) |
| H17B | 0.2830 | -0.1927 | 1.1340 | 0.073* | 0.573 (7) |
| C18' | 0.2375 (2) | -0.0777 (12) | 1.2611 (6) | 0.0409 (13) | 0.573 (7) |
| H18A | 0.2612 | 0.0151 | 1.2993 | 0.049* | 0.573 (7) |
| H18B | 0.2295 | -0.1906 | 1.3353 | 0.049* | 0.573 (7) |
| N1 | 0.15384 (7) | 0.4150 (4) | 1.0215 (3) | 0.0303 (5) | |
| N2 | 0.17893 (8) | 0.2525 (4) | 0.9464 (3) | 0.0326 (5) | |
| S1 | 0.23331 (2) | -0.09801 (13) | 0.96398 (8) | 0.0371 (2) | |
| S2 | 0.19208 (2) | 0.10941 (13) | 1.22517 (8) | 0.03412 (18) | |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-----------|-------------|-------------|--------------|--------------|
| C1 | 0.0449 (17) | 0.054 (2) | 0.0529 (19) | 0.0162 (16) | -0.0127 (17) | -0.0014 (18) |
| C2 | 0.0450 (18) | 0.064 (3) | 0.062 (2) | 0.025 (2) | -0.0003 (18) | 0.011 (2) |
| C3 | 0.0468 (19) | 0.048 (2) | 0.063 (2) | 0.0138 (16) | 0.0177 (17) | 0.0037 (17) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C4 | 0.0448 (17) | 0.057 (2) | 0.062 (2) | 0.0032 (17) | 0.0105 (19) | -0.014 (2) |
| C5 | 0.0282 (14) | 0.0498 (19) | 0.0489 (19) | 0.0002 (14) | 0.0035 (13) | -0.0052 (15) |
| C6 | 0.0304 (13) | 0.0307 (15) | 0.0353 (14) | 0.0037 (12) | 0.0044 (11) | 0.0105 (12) |
| C7 | 0.0307 (13) | 0.0326 (14) | 0.0321 (13) | -0.0017 (12) | -0.0014 (12) | 0.0042 (13) |
| C8 | 0.0300 (12) | 0.0319 (15) | 0.0287 (13) | 0.0000 (12) | 0.0000 (10) | 0.0062 (11) |
| C9 | 0.0245 (12) | 0.0292 (14) | 0.0326 (14) | -0.0031 (11) | 0.0000 (10) | 0.0083 (11) |
| C10 | 0.0256 (12) | 0.0277 (14) | 0.0328 (13) | 0.0085 (11) | 0.0001 (11) | 0.0060 (11) |
| C11 | 0.0465 (16) | 0.0330 (16) | 0.0405 (18) | 0.0057 (14) | -0.0028 (14) | 0.0068 (14) |
| C12 | 0.061 (2) | 0.0419 (19) | 0.0426 (18) | 0.0144 (18) | -0.0111 (16) | -0.0071 (15) |
| C13 | 0.0507 (18) | 0.056 (2) | 0.0300 (14) | 0.0256 (17) | 0.0009 (16) | 0.0032 (16) |
| C14 | 0.0417 (16) | 0.050 (2) | 0.0358 (16) | 0.0093 (16) | 0.0069 (14) | 0.0178 (15) |
| C15 | 0.0303 (13) | 0.0381 (17) | 0.0373 (16) | 0.0033 (13) | 0.0026 (11) | 0.0097 (13) |
| C16 | 0.0260 (12) | 0.0276 (15) | 0.0266 (12) | -0.0049 (11) | -0.0006 (10) | 0.0055 (11) |
| C17 | 0.087 (6) | 0.050 (6) | 0.046 (2) | 0.039 (5) | -0.018 (3) | -0.001 (3) |
| C18 | 0.038 (3) | 0.039 (4) | 0.046 (3) | 0.009 (2) | -0.016 (2) | 0.008 (3) |
| C17' | 0.087 (6) | 0.050 (6) | 0.046 (2) | 0.039 (5) | -0.018 (3) | -0.001 (3) |
| C18' | 0.038 (3) | 0.039 (4) | 0.046 (3) | 0.009 (2) | -0.016 (2) | 0.008 (3) |
| N1 | 0.0260 (11) | 0.0347 (13) | 0.0302 (11) | 0.0046 (10) | 0.0023 (9) | 0.0081 (10) |
| N2 | 0.0315 (11) | 0.0357 (13) | 0.0306 (12) | 0.0058 (10) | 0.0038 (9) | 0.0078 (10) |
| S1 | 0.0372 (4) | 0.0369 (4) | 0.0373 (4) | 0.0088 (3) | 0.0046 (3) | 0.0062 (4) |
| S2 | 0.0336 (3) | 0.0405 (4) | 0.0283 (3) | 0.0076 (3) | -0.0037 (3) | 0.0034 (3) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|-----------|-----------|
| C1—C2 | 1.389 (5) | C13—C14 | 1.373 (5) |
| C1—C6 | 1.404 (4) | C13—H13 | 0.9300 |
| C1—H1 | 0.9300 | C14—C15 | 1.391 (4) |
| C2—C3 | 1.362 (6) | C14—H14 | 0.9300 |
| C2—H2 | 0.9300 | C15—H15 | 0.9300 |
| C3—C4 | 1.381 (5) | C16—N2 | 1.284 (3) |
| C3—H3 | 0.9300 | C16—S1 | 1.736 (3) |
| C4—C5 | 1.383 (5) | C16—S2 | 1.765 (3) |
| C4—H4 | 0.9300 | C17—C18 | 1.406 (5) |
| C5—C6 | 1.378 (4) | C17—S1 | 1.750 (5) |
| C5—H5 | 0.9300 | C17—H17C | 0.9700 |
| C6—C7 | 1.471 (4) | C17—H17D | 0.9700 |
| C7—C8 | 1.334 (4) | C18—S2 | 1.839 (8) |
| C7—H7 | 0.9300 | C18—H18C | 0.9700 |
| C8—C9 | 1.451 (4) | C18—H18D | 0.9700 |
| C8—H8 | 0.9300 | C17'—C18' | 1.410 (5) |
| C9—N1 | 1.296 (3) | C17'—S1 | 1.759 (4) |
| C9—C10 | 1.489 (4) | C17'—H17A | 0.9700 |
| C10—C11 | 1.390 (5) | C17'—H17B | 0.9700 |
| C10—C15 | 1.397 (4) | C18'—S2 | 1.798 (5) |
| C11—C12 | 1.382 (5) | C18'—H18A | 0.9700 |
| C11—H11 | 0.9300 | C18'—H18B | 0.9700 |
| C12—C13 | 1.378 (5) | N1—N2 | 1.394 (3) |
| C12—H12 | 0.9300 | | |

| | | | |
|-------------|-----------|----------------|-------------|
| C2—C1—C6 | 119.8 (4) | C13—C14—C15 | 120.5 (3) |
| C2—C1—H1 | 120.1 | C13—C14—H14 | 119.7 |
| C6—C1—H1 | 120.1 | C15—C14—H14 | 119.7 |
| C3—C2—C1 | 121.3 (3) | C14—C15—C10 | 120.0 (3) |
| C3—C2—H2 | 119.4 | C14—C15—H15 | 120.0 |
| C1—C2—H2 | 119.4 | C10—C15—H15 | 120.0 |
| C2—C3—C4 | 119.3 (3) | N2—C16—S1 | 120.0 (2) |
| C2—C3—H3 | 120.3 | N2—C16—S2 | 124.7 (2) |
| C4—C3—H3 | 120.3 | S1—C16—S2 | 115.30 (15) |
| C3—C4—C5 | 120.0 (4) | C18—C17—S1 | 113.9 (6) |
| C3—C4—H4 | 120.0 | C18—C17—H17C | 108.8 |
| C5—C4—H4 | 120.0 | S1—C17—H17C | 108.8 |
| C6—C5—C4 | 121.5 (3) | C18—C17—H17D | 108.8 |
| C6—C5—H5 | 119.2 | S1—C17—H17D | 108.8 |
| C4—C5—H5 | 119.2 | H17C—C17—H17D | 107.7 |
| C5—C6—C1 | 118.0 (3) | C17—C18—S2 | 117.1 (6) |
| C5—C6—C7 | 122.9 (3) | C17—C18—H18C | 108.0 |
| C1—C6—C7 | 119.1 (3) | S2—C18—H18C | 108.0 |
| C8—C7—C6 | 126.1 (3) | C17—C18—H18D | 108.0 |
| C8—C7—H7 | 117.0 | S2—C18—H18D | 108.0 |
| C6—C7—H7 | 117.0 | H18C—C18—H18D | 107.3 |
| C7—C8—C9 | 125.3 (3) | C18'—C17'—S1 | 118.1 (5) |
| C7—C8—H8 | 117.3 | C18'—C17'—H17A | 107.8 |
| C9—C8—H8 | 117.3 | S1—C17'—H17A | 107.8 |
| N1—C9—C8 | 115.8 (2) | C18'—C17'—H17B | 107.8 |
| N1—C9—C10 | 124.4 (3) | S1—C17'—H17B | 107.8 |
| C8—C9—C10 | 119.8 (2) | H17A—C17'—H17B | 107.1 |
| C11—C10—C15 | 118.6 (3) | C17'—C18'—S2 | 112.4 (5) |
| C11—C10—C9 | 121.7 (3) | C17'—C18'—H18A | 109.1 |
| C15—C10—C9 | 119.7 (3) | S2—C18'—H18A | 109.1 |
| C12—C11—C10 | 120.6 (4) | C17'—C18'—H18B | 109.1 |
| C12—C11—H11 | 119.7 | S2—C18'—H18B | 109.1 |
| C10—C11—H11 | 119.7 | H18A—C18'—H18B | 107.8 |
| C13—C12—C11 | 120.5 (4) | C9—N1—N2 | 114.7 (2) |
| C13—C12—H12 | 119.8 | C16—N2—N1 | 112.1 (2) |
| C11—C12—H12 | 119.8 | C16—S1—C17 | 98.9 (3) |
| C14—C13—C12 | 119.7 (3) | C16—S1—C17' | 95.7 (3) |
| C14—C13—H13 | 120.1 | C16—S2—C18' | 95.8 (2) |
| C12—C13—H13 | 120.1 | C16—S2—C18 | 93.4 (3) |

Hydrogen-bond geometry (Å, °)

| <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> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| C17'—H17B...Cg ⁱ | 0.97 | 2.94 | 3.842 (9) | 156 |

| | | | | |
|------------------------------|------|------|-----------|-----|
| C18'—H18A···S1 ⁱⁱ | 0.97 | 2.69 | 3.439 (6) | 135 |
| C18'—H18B···S1 ⁱ | 0.97 | 2.86 | 3.628 (7) | 137 |

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