

rac-cis-5-Methyl-2,3-diphenyl-1,3-thiazolidin-4-one

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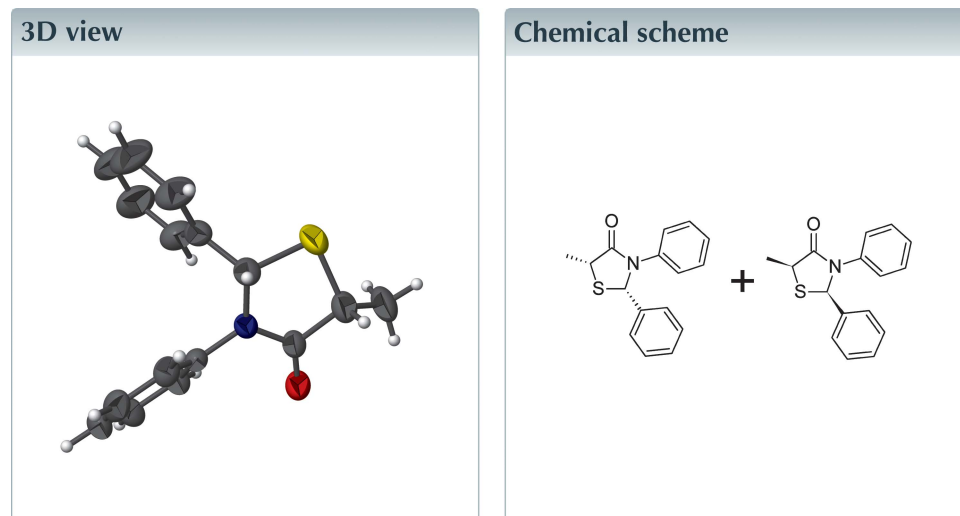
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Structural data: full structural data are available from iucrdata.iucr.org

In the racemic title compound, C₁₆H₁₅NOS, the thiazolidine ring adopts an envelope conformation, with the S atom as the flap. The dihedral angles between the heterocycle (all atoms) and pendant C- and N-bound benzene rings are 69.75 (14) and 56.56 (11)°, respectively; the aromatic rings are almost orthogonal to each other, with a dihedral angle of 76.04 (14)° between them. In the crystal, molecules are linked by weak C—H···O hydrogen bonds to generate [101] chains, with alternating molecules being enantiomers. A weak C—H···π interaction is also observed.



Structure description

1,3-Thiazolidin-4-ones are of great interest due to their high and diverse biological activity (Jain *et al.*, 2012). 5-Methyl-2,3-diaryl-1,3-thiazolidinones are readily available by use of thiolactic acid in the preparation (Patel *et al.*, 1976) and show antimicrobial activity (Piscopo *et al.*, 1988; Piscopo, Diurno, Gagliardi, Mazzoni, Parrilli & Veneruso, 1989; Piscopo, Diurno, Gagliardi, Mazzoni, De Francesco & Veneruso, 1989; Piscopo, Diurno, Gagliardi, Mazzoni & Veneruso, 1989). However, while the crystal structures of a number of 5-methyl-1,3-thiazolidin-4-ones have been reported (Rang *et al.*, 1997; Öztürk *et al.*, 2000; Dandia *et al.*; 2006; Yalçın *et al.*, 2008; Akkurt *et al.*, 2010, 2011, 2012; Ostapiuk *et al.*, 2012; Jiang *et al.*, 2012), only two of them were 2,3-diaryl substituted (Öztürk *et al.*, 2000; Dandia *et al.*; 2006).

Herein, we report the synthesis and crystal structure of the *cis* isomer of *rac*-5-methyl-2,3-diphenyl-1,3-thiazolidin-4-one. Woolston *et al.* (1993) have reported observing a 3:1 *cis:trans* ratio in the product, although the method of isolation was not specified. We have previously reported the structure of 2,3-diphenyl-1,3-thiazolidin-4-one (Yennawar *et al.*, 2014). The most closely related 5-methyl compound whose crystal structure is known is

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

Cg3 is the centroid of the C11–C16 ring.

<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>
C13–H13...O1 ⁱ	0.93	2.51	3.366 (3)	154
C3–H3...Cg3 ⁱⁱ	0.98	2.90	3.783 (3)	151

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

the 3-(*p*-chlorophenyl)-2-(8-quinolinyl) compound of Özturk *et al.* (2000), which displayed an envelope conformation for the thiazolidinone ring.

The title compound (Fig. 1) shows an envelope conformation for the five-membered 1,3-thiazolidin-4-one ring with substitutions at the 2, 3, and 5 ring positions. The phenyl rings at the 2 and 3 positions are close to orthogonal to each other with a dihedral angle of 76.04 (14)° between their planes. In the arbitrarily chosen asymmetric molecule (Fig. 1), C1 and C3 have *S* and *R* configurations, respectively, but crystal symmetry generates a racemic mixture. In the extended structure (Fig. 2), the oxygen atom connected to the 4 position of the heterocycle accepts a C–H...O interaction (Table 1) arising from a phenyl ring at the 3 position of a symmetry-related enantiomer, resulting in a chain-link in the [101] direction. A weak C–H...O interaction (Table 1) is also observed.

Synthesis and crystallization

0.05 mol of *N*-benzylideneaniline and a slight excess of thioctic acid were dissolved in 60 ml of toluene in a 100 ml round-

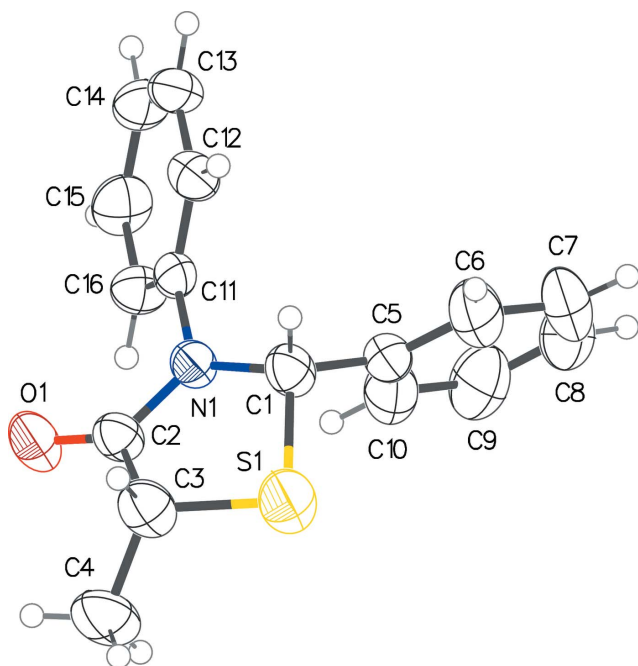


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₅ NOS
<i>M_r</i>	269.35
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.2271 (16), 22.531 (6), 9.937 (3)
β (°)	96.545 (4)
<i>V</i> (Å ³)	1385.1 (6)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.23
Crystal size (mm)	0.15 × 0.1 × 0.09
Data collection	
Diffractometer	Bruker <i>SAINT</i> CCD area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2001)
<i>T_{min}</i> , <i>T_{max}</i>	0.838, 0.9
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	10624, 3360, 2378
<i>R_{int}</i>	0.037
(sin θ/λ) _{max} (Å ⁻¹)	0.668
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.063, 0.171, 1.04
No. of reflections	3360
No. of parameters	173
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.46, -0.18

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009) and *pubCIF* (Westrip, 2010).

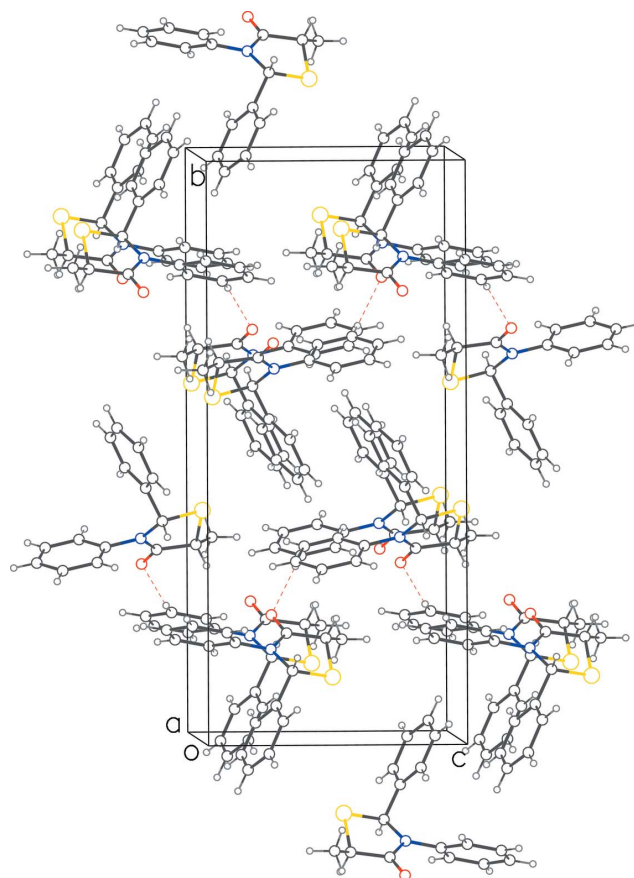


Figure 2
Packing diagram of the title compound, with red dotted lines representing C–H...O contacts forming chains propagating in the [101] direction.

bottomed flask. The flask was connected to a Dean–Stark trap and condenser and refluxed for 6 h. After cooling, the excess thiolactic acid was neutralized with 5% aqueous NaHCO₃ solution. The toluene layer was removed under vacuum on a rotary evaporator. The product was recrystallized from 95% ethanol solution: m.p. 391–393 K (no literature reports). Crystals for X-ray diffraction studies were grown by slow evaporation from ethanol solution. Only the *cis* isomer was isolated.

Refinement

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

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References

- Akkurt, M., Çelik, İ., Demir, H., Özkırımlı, S. & Büyükgüngör, O. (2011). *Acta Cryst.* **E67**, o293–o294.
- Akkurt, M., Gürsoy, E., Güzeldemirci, N. U., Türktekin-Çelikesir, S. & Tahir, M. N. (2012). *Acta Cryst.* **E68**, o1505–o1506.
- Akkurt, M., Nassozi, M., Kocabalkanlı, A., Khan, I. U. & Sharif, S. (2010). *Acta Cryst.* **E66**, o882.
- Bruker (2001). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dandia, A., Singh, R., Khaturia, S., Mérienne, C., Morgant, G. & Loupy, A. (2006). *Bioorg. Med. Chem.* **14**, 2409–2417.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Jain, A. K., Vaidya, A., Ravichandran, V., Kashaw, S. K. & Agrawal, R. K. (2012). *Bioorg. Med. Chem.* **20**, 3378–3395.
- Jiang, J.-R., Xu, F., Ke, Z.-L. & Li, L. (2012). *Acta Cryst.* **E68**, o34.
- Ostapiuk, Y. V., Obushak, M. K., Matiychuk, V. S., Naskrent, M. & Gzella, A. K. (2012). *Tetrahedron Lett.* **53**, 543–545.
- Öztürk, S., Aygün, M., Öcal, N., Yolacan, C. III & Fun, H.-K. (2000). *NCS*, **215**, 526–528.
- Patel, D. R., Satpanthi, P. S., Patel, P. B. & Trivedi, J. J. (1976). *J. Inst. Chem. (India)*, **48**(6), 305–308.
- Piscopo, E., Diurno, M. V., Gagliardi, R., Mazzoni, O. & Aliberti, F. (1988). *Boll. Soc. Ital. Biol. Sper.* **64**, 153–158.
- Piscopo, E., Diurno, M. V., Gagliardi, R., Mazzoni, O., de Francesco, F. M. & Veneruso, G. (1989). *Boll. Soc. Ital. Biol. Sper.* **65**, 535–541.
- Piscopo, E., Diurno, M. V., Gagliardi, R., Mazzoni, O., Parrilli, C. & Veneruso, G. (1989). *Boll. Soc. Ital. Biol. Sper.* **65**, 131–136.
- Piscopo, E., Diurno, M. V., Gagliardi, R., Mazzoni, O. & Veneruso, G. (1989). *Boll. Soc. Ital. Biol. Sper.* **65**, 853–859.
- Rang, K., Liao, F.-L., Sandström, J. & Wang, S.-L. (1997). *Chirality*, **9**, 568–577.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Woolston, C. R. J., Lee, J. B. & Swinbourne, J. (1993). *Magn. Reson. Chem.* **31**, 348–351.
- Yalçın, Ş. P., Akkurt, M., Şahin, E., Güzel, Ö., Salman, A. & İhan, E. (2008). *Acta Cryst.* **E64**, o1919.
- Yennawar, H. P., Tierney, J. & Silverberg, L. J. (2014). *Acta Cryst.* **E70**, o847.

full crystallographic data

IUCrData (2017). 2, x171662 [https://doi.org/10.1107/S2414314617016625]

***rac-cis*-5-Methyl-2,3-diphenyl-1,3-thiazolidin-4-one**

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rac-cis*-5-Methyl-2,3-diphenyl-1,3-thiazolidin-4-oneCrystal data*

$C_{16}H_{15}NOS$

$M_r = 269.35$

Monoclinic, $P2_1/c$

$a = 6.2271$ (16) Å

$b = 22.531$ (6) Å

$c = 9.937$ (3) Å

$\beta = 96.545$ (4)°

$V = 1385.1$ (6) Å³

$Z = 4$

$F(000) = 568$

$D_x = 1.292$ Mg m⁻³

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

Cell parameters from 2561 reflections

$\theta = 2.3$ – 25.6 °

$\mu = 0.23$ mm⁻¹

$T = 298$ K

Block, colorless

$0.15 \times 0.1 \times 0.09$ mm

Data collection

Bruker SAINT CCD area detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

$T_{\min} = 0.838$, $T_{\max} = 0.9$

10624 measured reflections

3360 independent reflections

2378 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 28.3$ °, $\theta_{\min} = 1.8$ °

$h = -8 \rightarrow 7$

$k = -30 \rightarrow 29$

$l = -12 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.171$

$S = 1.04$

3360 reflections

173 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

$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 0.3983P]$

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

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

$\Delta\rho_{\max} = 0.46$ e Å⁻³

$\Delta\rho_{\min} = -0.18$ e Å⁻³

Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 4 sets of ω scans each set at different ϕ and/or 2θ angles and each scan (30 s exposure) covering -0.300 ° degrees in ω . The crystal to detector distance was 5.82 cm.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.41425 (13)	0.39324 (4)	1.01291 (7)	0.0782 (3)
O1	0.7411 (3)	0.29432 (8)	0.80393 (16)	0.0588 (5)
N1	0.4230 (3)	0.34551 (7)	0.77525 (17)	0.0393 (4)
C1	0.2685 (4)	0.37863 (10)	0.8464 (2)	0.0476 (5)
H1	0.1414	0.3540	0.8557	0.057*
C2	0.5992 (3)	0.32204 (10)	0.8504 (2)	0.0440 (5)
C3	0.5912 (4)	0.33075 (12)	1.0016 (2)	0.0568 (6)
H3	0.5222	0.2958	1.0365	0.068*
C4	0.8088 (5)	0.33802 (15)	1.0804 (3)	0.0754 (8)
H4A	0.8720	0.3747	1.0556	0.113*
H4B	0.9003	0.3056	1.0608	0.113*
H4C	0.7939	0.3384	1.1755	0.113*
C5	0.1991 (4)	0.43677 (10)	0.7778 (2)	0.0490 (6)
C6	-0.0051 (5)	0.45857 (14)	0.7878 (4)	0.0784 (9)
H6	-0.1011	0.4371	0.8341	0.094*
C7	-0.0674 (6)	0.51299 (16)	0.7282 (5)	0.0978 (12)
H7	-0.2034	0.5285	0.7374	0.117*
C8	0.0701 (6)	0.54313 (13)	0.6571 (4)	0.0914 (11)
H8	0.0259	0.5785	0.6144	0.110*
C9	0.2736 (6)	0.52196 (13)	0.6475 (4)	0.0880 (10)
H9	0.3688	0.5433	0.6005	0.106*
C10	0.3364 (5)	0.46888 (11)	0.7080 (3)	0.0674 (7)
H10	0.4748	0.4545	0.7012	0.081*
C11	0.3725 (3)	0.33221 (8)	0.6344 (2)	0.0364 (4)
C12	0.1711 (3)	0.31056 (9)	0.5866 (2)	0.0461 (5)
H12	0.0676	0.3043	0.6456	0.055*
C13	0.1239 (4)	0.29816 (10)	0.4495 (3)	0.0549 (6)
H13	-0.0110	0.2830	0.4171	0.066*
C14	0.2734 (5)	0.30799 (11)	0.3619 (2)	0.0587 (7)
H14	0.2396	0.3002	0.2700	0.070*
C15	0.4750 (5)	0.32947 (11)	0.4101 (3)	0.0589 (6)
H15	0.5777	0.3356	0.3505	0.071*
C16	0.5252 (4)	0.34184 (10)	0.5455 (2)	0.0471 (5)
H16	0.6610	0.3566	0.5774	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0871 (6)	0.1043 (6)	0.0412 (4)	0.0397 (4)	-0.0008 (3)	-0.0177 (3)
O1	0.0519 (10)	0.0811 (12)	0.0429 (9)	0.0258 (8)	0.0034 (7)	0.0011 (8)
N1	0.0373 (9)	0.0469 (9)	0.0335 (9)	0.0062 (7)	0.0036 (7)	-0.0016 (7)
C1	0.0421 (12)	0.0592 (13)	0.0418 (12)	0.0086 (10)	0.0067 (9)	-0.0020 (10)
C2	0.0423 (12)	0.0532 (12)	0.0357 (11)	0.0045 (9)	0.0017 (9)	0.0013 (9)
C3	0.0554 (15)	0.0754 (16)	0.0396 (12)	0.0111 (12)	0.0050 (11)	0.0025 (11)
C4	0.0681 (18)	0.114 (2)	0.0408 (14)	0.0151 (16)	-0.0070 (13)	-0.0096 (14)
C5	0.0447 (12)	0.0516 (13)	0.0492 (13)	0.0081 (10)	-0.0018 (10)	-0.0094 (10)
C6	0.0573 (17)	0.0719 (18)	0.106 (3)	0.0172 (14)	0.0090 (16)	-0.0056 (17)
C7	0.071 (2)	0.077 (2)	0.140 (4)	0.0350 (18)	-0.011 (2)	-0.007 (2)
C8	0.102 (3)	0.0477 (15)	0.116 (3)	0.0148 (17)	-0.024 (2)	-0.0010 (16)
C9	0.104 (3)	0.0518 (16)	0.108 (3)	0.0031 (16)	0.010 (2)	0.0053 (16)
C10	0.0656 (17)	0.0515 (14)	0.085 (2)	0.0066 (12)	0.0094 (15)	0.0011 (13)
C11	0.0397 (11)	0.0332 (9)	0.0355 (10)	0.0045 (8)	0.0005 (8)	0.0008 (8)
C12	0.0404 (12)	0.0484 (12)	0.0484 (13)	0.0003 (9)	-0.0005 (10)	0.0058 (9)
C13	0.0519 (14)	0.0490 (12)	0.0580 (15)	-0.0020 (10)	-0.0183 (12)	-0.0003 (11)
C14	0.0752 (18)	0.0578 (14)	0.0395 (12)	0.0074 (12)	-0.0096 (12)	-0.0077 (10)
C15	0.0683 (17)	0.0684 (15)	0.0415 (13)	0.0031 (12)	0.0130 (12)	-0.0035 (11)
C16	0.0452 (12)	0.0560 (13)	0.0396 (11)	-0.0043 (10)	0.0031 (10)	-0.0019 (10)

Geometric parameters (Å, °)

S1—C1	1.824 (2)	C7—H7	0.9300
S1—C3	1.799 (3)	C7—C8	1.354 (5)
O1—C2	1.216 (3)	C8—H8	0.9300
N1—C1	1.461 (3)	C8—C9	1.367 (5)
N1—C2	1.362 (3)	C9—H9	0.9300
N1—C11	1.431 (3)	C9—C10	1.375 (4)
C1—H1	0.9800	C10—H10	0.9300
C1—C5	1.517 (3)	C11—C12	1.379 (3)
C2—C3	1.521 (3)	C11—C16	1.387 (3)
C3—H3	0.9800	C12—H12	0.9300
C3—C4	1.495 (4)	C12—C13	1.389 (3)
C4—H4A	0.9600	C13—H13	0.9300
C4—H4B	0.9600	C13—C14	1.363 (4)
C4—H4C	0.9600	C14—H14	0.9300
C5—C6	1.377 (3)	C14—C15	1.379 (4)
C5—C10	1.367 (4)	C15—H15	0.9300
C6—H6	0.9300	C15—C16	1.375 (3)
C6—C7	1.397 (5)	C16—H16	0.9300
C3—S1—C1	92.68 (11)	C6—C7—H7	120.0
C2—N1—C1	117.80 (17)	C8—C7—C6	120.0 (3)
C2—N1—C11	121.92 (17)	C8—C7—H7	120.0
C11—N1—C1	119.78 (16)	C7—C8—H8	119.7

S1—C1—H1	109.9	C7—C8—C9	120.5 (3)
N1—C1—S1	104.13 (14)	C9—C8—H8	119.7
N1—C1—H1	109.9	C8—C9—H9	120.2
N1—C1—C5	113.16 (18)	C8—C9—C10	119.5 (3)
C5—C1—S1	109.79 (16)	C10—C9—H9	120.2
C5—C1—H1	109.9	C5—C10—C9	121.2 (3)
O1—C2—N1	124.5 (2)	C5—C10—H10	119.4
O1—C2—C3	123.3 (2)	C9—C10—H10	119.4
N1—C2—C3	112.13 (19)	C12—C11—N1	120.07 (18)
S1—C3—H3	108.1	C12—C11—C16	119.9 (2)
C2—C3—S1	104.59 (16)	C16—C11—N1	120.02 (19)
C2—C3—H3	108.1	C11—C12—H12	120.3
C4—C3—S1	114.0 (2)	C11—C12—C13	119.4 (2)
C4—C3—C2	113.7 (2)	C13—C12—H12	120.3
C4—C3—H3	108.1	C12—C13—H13	119.7
C3—C4—H4A	109.5	C14—C13—C12	120.7 (2)
C3—C4—H4B	109.5	C14—C13—H13	119.7
C3—C4—H4C	109.5	C13—C14—H14	120.1
H4A—C4—H4B	109.5	C13—C14—C15	119.8 (2)
H4A—C4—H4C	109.5	C15—C14—H14	120.1
H4B—C4—H4C	109.5	C14—C15—H15	119.8
C6—C5—C1	119.6 (2)	C16—C15—C14	120.5 (2)
C10—C5—C1	121.5 (2)	C16—C15—H15	119.8
C10—C5—C6	118.9 (2)	C11—C16—H16	120.1
C5—C6—H6	120.1	C15—C16—C11	119.7 (2)
C5—C6—C7	119.8 (3)	C15—C16—H16	120.1
C7—C6—H6	120.1		
S1—C1—C5—C6	-94.9 (3)	C2—N1—C11—C12	125.9 (2)
S1—C1—C5—C10	83.8 (3)	C2—N1—C11—C16	-54.9 (3)
O1—C2—C3—S1	160.9 (2)	C3—S1—C1—N1	-24.32 (17)
O1—C2—C3—C4	35.9 (4)	C3—S1—C1—C5	-145.76 (17)
N1—C1—C5—C6	149.2 (2)	C5—C6—C7—C8	2.2 (5)
N1—C1—C5—C10	-32.1 (3)	C6—C5—C10—C9	-0.4 (4)
N1—C2—C3—S1	-23.0 (2)	C6—C7—C8—C9	-2.7 (6)
N1—C2—C3—C4	-148.0 (2)	C7—C8—C9—C10	1.6 (6)
N1—C11—C12—C13	179.64 (18)	C8—C9—C10—C5	-0.1 (5)
N1—C11—C16—C15	-179.4 (2)	C10—C5—C6—C7	-0.6 (4)
C1—S1—C3—C2	26.91 (18)	C11—N1—C1—S1	-172.77 (15)
C1—S1—C3—C4	151.7 (2)	C11—N1—C1—C5	-53.6 (3)
C1—N1—C2—O1	-178.9 (2)	C11—N1—C2—O1	9.2 (3)
C1—N1—C2—C3	5.0 (3)	C11—N1—C2—C3	-166.80 (19)
C1—N1—C11—C12	-45.7 (3)	C11—C12—C13—C14	-1.0 (3)
C1—N1—C11—C16	133.4 (2)	C12—C11—C16—C15	-0.3 (3)
C1—C5—C6—C7	178.1 (3)	C12—C13—C14—C15	1.2 (4)
C1—C5—C10—C9	-179.1 (3)	C13—C14—C15—C16	-0.9 (4)
C2—N1—C1—S1	15.2 (2)	C14—C15—C16—C11	0.5 (4)
C2—N1—C1—C5	134.4 (2)	C16—C11—C12—C13	0.5 (3)

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C11–C16 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C13—H13 \cdots O1 ⁱ	0.93	2.51	3.366 (3)	154
C3—H3 \cdots Cg3 ⁱⁱ	0.98	2.90	3.783 (3)	151

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