Crystal structure of rac-2,3-diphenyl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-one 1-oxide

Hemant P. Yennawar,[a] Ziwei Yang[b] and Lee J. Silverberg[b]*

[a]Department of Biochemistry and Molecular Biology, Pennsylvania State University, University Park, PA 16802, USA, and [b]Pennsylvania State University, Schuylkill Campus, 200 University Drive, Schuylkill Haven, PA 17972, USA. *Correspondence e-mail: ljs43@psu.edu

In the title compound, $C_{16}H_{15}NO_2S$ [alternative name: rac-2,3-diphenyl-1,3-thiazinan-4-one 1-oxide], the thiazine ring exhibits an envelope conformation, with the S atom forming the flap. The sulfoxide O atom is in a pseudo-axial position on the thiazine ring and is trans to the phenyl group on C-2. The phenyl rings form a dihedral angle of 89.47 (19)°. In this racemate crystal, homochiral molecules form slabs parallel to (010) of thickness b/2 which then stack with alternating chirality in the b-axis direction. The stacking is aided by edge-to-face interactions between the phenyl rings of racemic molecules. Within each of the single-enantiomer slabs, the molecules are held by C—H···O-type interactions, with an H···O distance of 2.30 Å, forming infinite chains along the c-axis direction, as well by the edge-to-face interactions between phenyl rings of neighboring molecules in the a-axis direction.

1. Chemical context

1,3-Thiazin-4-ones are a group of six-membered heterocycles with a wide range of biological activity (Ryabukhin et al., 1996). Surrey's research (Surrey et al., 1958; Surrey, 1963a) resulted in the discovery of two drugs, the anti-anxiety and muscle relaxant chlormezanone [2-(4-chlorophenyl)-3-methyl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-one 1,1-dioxide; Merck Index, 2006; Tanaka & Hirayama, 2005] and muscle relaxant dichlormezanone [2-(3,4-dichlorophenyl)-3-methyl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-one 1,1-dioxide; Dictionary of Drugs, 1990]. These sulfones showed greater activity than the sulfides from which they were synthesized (Surrey et al., 1958). Surrey also prepared a variety of other sulfoxides and sulfones of 3-alkyl-2-aryl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-ones (Surrey, 1963a,b). Surrey did not successfully synthesize any 2-aryl-3-aryl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-ones (Silverberg et al., 2015), and to the best of our knowledge nobody has reported any oxides of this type of compound. We previously reported the crystal structure of 2,3-diphenyl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-one (Yennawar & Silverberg, 2014). Herein, we report the crystal structure of that compound's sulfoxide, prepared using the method we have previously reported for oxidation of the five-membered 1,3-thiazolidin-4-ones (Cannon et al., 2015).

2. Structural commentary

The crystal structure of this racemic compound shows a thiazine ring in an envelope pucker with puckering amplitude of 0.718 (3) Å (Fig. 1). The oxygen on sulfur is pseudo-axial on
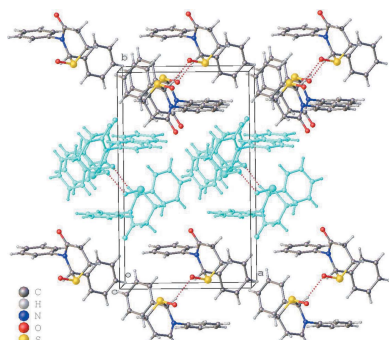
the thiazine ring. The two phenyl rings, on two adjacent atoms of the thiazine ring, are perpendicular to each other with an angle of 89.47 (19)° between their planes. The oxygen on sulfur and the phenyl ring on C2 are *trans* to each other.
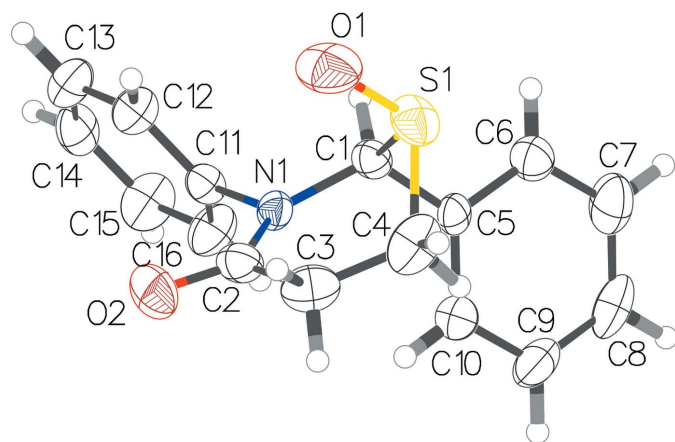
crystal structures of a 2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one 1-oxide.
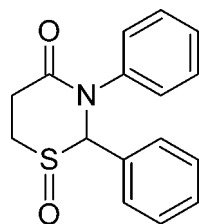
3. Supramolecular features

The crystal consists of a racemic mixture of the title compound. The two phenyl groups and one of the two oxygen atoms participate in intermolecular interactions (Table 1). The molecules of single chirality form slabs in the *ac* plane aided by π–π edge-to-face interactions, with inter-centroid distance of 5.195 (3) Å, in the *a*-axis direction and with C—H$\cdots$O hydrogen-bonds (Table 1) in the *c*-axis direction (Fig. 2). Along the *b*-axis direction, these slabs stack with alternating chirality, stabilized once again by π–π edge-to-face interactions with inter-centroid distances of 5.021 (3) Å.

4. Database survey

Crystal structures of a number of 1,3-thiazolidin-4-one 1-oxides have been reported (Wang *et al.*, 2010; Johnson *et al.*, 1983; Chen *et al.*, 2011; Colombo *et al.*, 2008; Yennawar *et al.*, 2015); in each case the oxygen on sulfur and the group on C-2 had a *trans* relationship, as does the structure reported here. The structure of chlormezanone [2-(4-chlorophenyl)-3-methyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one 1,1-dioxide] has also been disclosed (Tanaka & Horayama, 2005). To the best of our knowledge, there have been no published

5. Synthesis and crystallization

A 5 mL round-bottom flask was charged with 50.5 mg of 2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one and 1.5 mL of methanol and stirred. A solution of 85.6 mg Oxone® and 0.74 mL distilled water was added dropwise and the mixture was stirred until the reaction was complete as determined by TLC. The solids were dissolved by addition of 7.4 mL distilled water. The solution was extracted with 7.4 mL dichloromethane. The organic layer was washed with distilled water and then with sat. sodium chloride. The solution was dried over Na_2SO_4 and concentrated under vacuum to a crude solid. This was chromatographed on flash silica gel, eluting with 70% ethyl acetate/hexanes, 100% ethyl acetate, and 100% acetone, giving 37.5 mg product (70% yield), m.p.: 396–400 K, $R_f = 0.23$ (EtOAc). Crystals for X-ray crystallography were grown by slow evaporation from ethanol solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were placed

Figure 1
The molecular conformation and atom-numbering scheme for the title compound, with non-H atoms shown as 50% probability displacement ellipsoids.
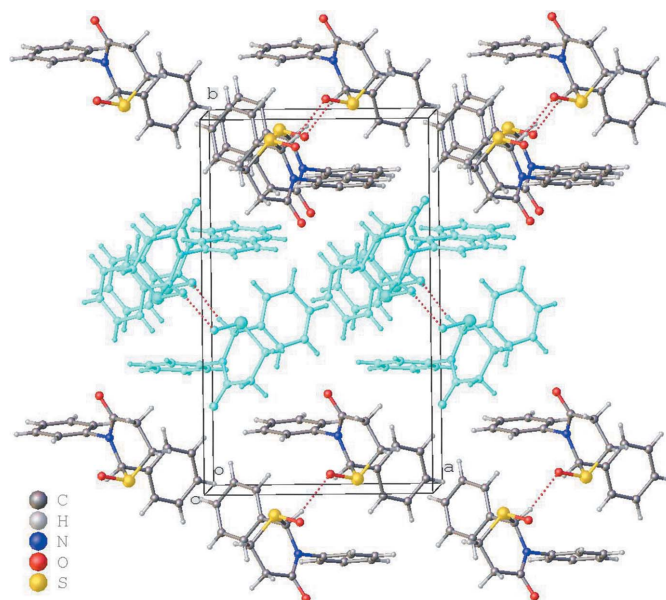
Figure 2
Packing viewed down the *c* axis. Alternating slabs of enantiomers along the *b*-axis direction are differentiated by the color scheme.

geometrically and allowed to ride on the carbon atoms during refinement, with C—H distances of 0.98 Å (methine), 0.96 Å (methyl) and 0.93 Å (aromatic) and with $U_{iso}(H) = 1.2U_{eq}$(aromatic and methine C) or $1.5U_{eq}$(methyl).

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{15}NO_2S$
M_r	285.35
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	298
a, b, c (Å)	10.547 (4), 17.317 (6), 7.592 (3)
V (Å^3)	1386.5 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	$0.23 \times 0.18 \times 0.16$
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.636, 0.964
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11124, 3428, 3182
R_{int}	0.032
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.075, 0.161, 1.26
No. of reflections	3428
No. of parameters	181
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.38, −0.27
Absolute structure	Flack (1983), 4716 Friedel pairs
Absolute structure parameter	0.12 (14)

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Crystal structure of *rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one 1-oxide

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Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

rac-2,3-Diphenyl-2,3,5,6-tetrahydro-4H-1,3-thiazin-4-one 1-oxide

Crystal data

$C_{16}H_{15}NO_2S$	$D_x = 1.367$ Mg m^{-3}
$M_r = 285.35$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $Pna2_1$	Cell parameters from 3661 reflections
$a = 10.547$ (4) Å	$\theta = 2.3$–26.4°
$b = 17.317$ (6) Å	$\mu = 0.23$ mm^{-1}
$c = 7.592$ (3) Å	$T = 298$ K
$V = 1386.5$ (8) Å^3	Block, colorless
$Z = 4$	$0.23 \times 0.18 \times 0.16$ mm
$F(000) = 600$	

Data collection

Bruker SMART APEX CCD area detector diffractometer	11124 measured reflections
Radiation source: fine-focus sealed tube	3428 independent reflections
Parallel,graphite monochromator	3182 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.032$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$\theta_{max} = 28.3°$, $\theta_{min} = 2.3°$
	$h = -13 \rightarrow 13$
	$k = -20 \rightarrow 23$
$T_{min} = 0.636$, $T_{max} = 0.964$	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.075$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.161$	
$S = 1.26$	H-atom parameters constrained
3428 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.8049P]$ where $P = (F_o^2 + 2F_c^2)/3$
181 parameters	
1 restraint	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.38$ e Å^{-3}
	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Absolute structure: Flack (1983), 4716 Friedel pairs

Absolute structure parameter: 0.12 (14)

Special details

Experimental. 1. SADABS was used for absorption correction. R(int) was 0.0424 before and 0.0268 after correction. The Ratio of minimum to maximum transmission is 0.6364. The $\lambda/2$ correction factor is 0.0015.

2. 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 (5 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 $F^2 > 2\text{sigma}(F^2)$ 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)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.17133 (10)	0.45935 (5)	−1.97816 (14)	0.0469 (3)
O1	0.0575 (3)	0.44303 (18)	−1.8700 (4)	0.0659 (9)
O2	0.0431 (3)	0.23452 (16)	−2.0769 (4)	0.0542 (8)
N1	0.0796 (2)	0.34956 (15)	−2.2011 (4)	0.0281 (6)
C1	0.1326 (3)	0.42779 (19)	−2.2029 (4)	0.0304 (7)
H1	0.0646	0.4619	−2.2442	0.036*
C2	0.1038 (4)	0.2938 (2)	−2.0808 (5)	0.0375 (8)
C3	0.2109 (4)	0.3050 (2)	−1.9494 (5)	0.0483 (10)
H3A	0.1771	0.2936	−1.8334	0.058*
H3B	0.2745	0.2660	−1.9744	0.058*
C4	0.2783 (4)	0.3813 (3)	−1.9375 (5)	0.0521 (11)
H4A	0.3465	0.3828	−2.0231	0.063*
H4B	0.3151	0.3870	−1.8211	0.063*
C5	0.2437 (3)	0.44151 (17)	−2.3232 (4)	0.0278 (6)
C6	0.2671 (4)	0.5164 (2)	−2.3791 (5)	0.0392 (8)
H6	0.2126	0.5559	−2.3446	0.047*
C7	0.3688 (4)	0.5333 (3)	−2.4840 (8)	0.0534 (10)
H7	0.3842	0.5839	−2.5186	0.064*
C8	0.4485 (4)	0.4748 (3)	−2.5384 (6)	0.0517 (11)
H8	0.5175	0.4860	−2.6103	0.062*
C9	0.4261 (3)	0.4006 (2)	−2.4869 (6)	0.0472 (9)
H9	0.4799	0.3613	−2.5247	0.057*
C10	0.3245 (3)	0.3830 (2)	−2.3791 (5)	0.0391 (8)
H10	0.3102	0.3323	−2.3441	0.047*
C11	−0.0254 (3)	0.33887 (18)	−2.3192 (4)	0.0297 (7)
C12	−0.1478 (4)	0.3459 (2)	−2.2599 (5)	0.0408 (8)
H12	−0.1627	0.3562	−2.1415	0.049*
C13	−0.2485 (4)	0.3378 (2)	−2.3733 (6)	0.0477 (10)

H13	−0.3313	0.3424	−2.3323	0.057*
C14	−0.2254 (4)	0.3231 (2)	−2.5468 (5)	0.0439 (9)
H14	−0.2934	0.3171	−2.6236	0.053*
C15	−0.1043 (4)	0.3169 (3)	−2.6103 (5)	0.0492 (10)
H15	−0.0901	0.3077	−2.7294	0.059*
C16	−0.0032 (4)	0.3244 (2)	−2.4953 (5)	0.0454 (9)
H16	0.0794	0.3197	−2.5366	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0600 (6)	0.0427 (5)	0.0380 (4)	−0.0080 (4)	0.0072 (5)	−0.0128 (4)
O1	0.083 (2)	0.0605 (18)	0.0548 (19)	0.0131 (17)	0.0259 (18)	−0.0026 (16)
O2	0.0614 (18)	0.0366 (15)	0.0648 (19)	−0.0055 (13)	0.0023 (15)	0.0188 (13)
N1	0.0242 (13)	0.0277 (13)	0.0325 (13)	−0.0015 (10)	0.0013 (12)	0.0054 (11)
C1	0.0326 (16)	0.0262 (15)	0.0323 (16)	0.0012 (13)	−0.0013 (14)	0.0026 (13)
C2	0.041 (2)	0.0306 (17)	0.0410 (19)	0.0064 (14)	0.0042 (16)	0.0056 (15)
C3	0.049 (2)	0.055 (2)	0.041 (2)	0.0142 (18)	−0.0079 (18)	0.0038 (18)
C4	0.042 (2)	0.080 (3)	0.034 (2)	−0.003 (2)	−0.0060 (16)	0.0044 (18)
C5	0.0233 (14)	0.0287 (14)	0.0316 (16)	−0.0045 (12)	−0.0070 (12)	0.0007 (13)
C6	0.0376 (19)	0.0357 (17)	0.0441 (19)	−0.0002 (15)	−0.0024 (16)	0.0036 (16)
C7	0.046 (2)	0.057 (2)	0.057 (2)	−0.0126 (18)	0.003 (3)	0.018 (2)
C8	0.0308 (19)	0.081 (3)	0.043 (2)	−0.017 (2)	0.0064 (16)	0.006 (2)
C9	0.0275 (16)	0.064 (2)	0.051 (2)	−0.0013 (16)	0.0053 (19)	−0.012 (2)
C10	0.0344 (19)	0.0370 (17)	0.046 (2)	−0.0008 (14)	−0.0017 (16)	−0.0019 (17)
C11	0.0333 (17)	0.0266 (14)	0.0293 (15)	0.0000 (12)	−0.0056 (14)	−0.0002 (13)
C12	0.0364 (19)	0.047 (2)	0.0388 (19)	−0.0003 (16)	0.0021 (15)	0.0013 (17)
C13	0.0287 (18)	0.055 (2)	0.059 (2)	−0.0006 (17)	0.0004 (18)	−0.002 (2)
C14	0.042 (2)	0.040 (2)	0.050 (2)	−0.0065 (16)	−0.0185 (17)	0.0007 (17)
C15	0.048 (2)	0.073 (3)	0.0261 (17)	−0.004 (2)	−0.0027 (17)	−0.0071 (18)
C16	0.0369 (18)	0.062 (2)	0.0374 (19)	−0.0022 (16)	0.0089 (17)	−0.0001 (19)

Geometric parameters (Å, º)

S1—O1	1.482 (3)	C5—C10	1.390 (5)
S1—C1	1.838 (4)	C6—C7	1.368 (6)
S1—C4	1.787 (5)	C7—C8	1.379 (6)
O2—C2	1.210 (5)	C8—C9	1.364 (6)
N1—C1	1.466 (4)	C9—C10	1.383 (5)
N1—C2	1.354 (4)	C11—C12	1.372 (5)
N1—C11	1.436 (4)	C11—C16	1.380 (5)
C1—C5	1.505 (5)	C12—C13	1.375 (6)
C2—C3	1.519 (5)	C13—C14	1.363 (6)
C3—C4	1.503 (6)	C14—C15	1.370 (6)
C5—C6	1.387 (5)	C15—C16	1.384 (6)
O1—S1—C1	106.12 (18)	C6—C5—C10	118.7 (3)
O1—S1—C4	105.8 (2)	C10—C5—C1	123.2 (3)

C4—S1—C1	94.34 (17)	C7—C6—C5	121.1 (4)
C2—N1—C1	126.4 (3)	C6—C7—C8	119.7 (4)
C2—N1—C11	118.4 (3)	C9—C8—C7	120.1 (4)
C11—N1—C1	114.0 (2)	C8—C9—C10	120.7 (4)
N1—C1—S1	110.6 (2)	C9—C10—C5	119.7 (3)
N1—C1—C5	116.7 (3)	C12—C11—N1	120.6 (3)
C5—C1—S1	110.1 (2)	C12—C11—C16	119.5 (3)
O2—C2—N1	121.4 (3)	C16—C11—N1	119.8 (3)
O2—C2—C3	119.0 (3)	C11—C12—C13	120.8 (4)
N1—C2—C3	119.5 (3)	C14—C13—C12	119.1 (4)
C4—C3—C2	120.2 (3)	C13—C14—C15	121.4 (4)
C3—C4—S1	110.9 (3)	C14—C15—C16	119.3 (4)
C6—C5—C1	118.1 (3)	C11—C16—C15	119.9 (3)
S1—C1—C5—C6	−76.3 (3)	C2—N1—C11—C16	−109.6 (4)
S1—C1—C5—C10	102.9 (3)	C2—C3—C4—S1	34.5 (4)
O1—S1—C1—N1	−49.2 (3)	C4—S1—C1—N1	58.6 (3)
O1—S1—C1—C5	−179.5 (2)	C4—S1—C1—C5	−71.7 (3)
O1—S1—C4—C3	46.9 (3)	C5—C6—C7—C8	1.3 (7)
O2—C2—C3—C4	−173.1 (4)	C6—C5—C10—C9	0.6 (5)
N1—C1—C5—C6	156.6 (3)	C6—C7—C8—C9	−0.3 (7)
N1—C1—C5—C10	−24.1 (4)	C7—C8—C9—C10	−0.5 (7)
N1—C2—C3—C4	8.0 (5)	C8—C9—C10—C5	0.3 (6)
N1—C11—C12—C13	178.2 (3)	C10—C5—C6—C7	−1.4 (6)
N1—C11—C16—C15	−177.7 (3)	C11—N1—C1—S1	139.1 (2)
C1—S1—C4—C3	−61.2 (3)	C11—N1—C1—C5	−94.1 (3)
C1—N1—C2—O2	170.2 (3)	C11—N1—C2—O2	3.5 (5)
C1—N1—C2—C3	−11.0 (5)	C11—N1—C2—C3	−177.6 (3)
C1—N1—C11—C12	−95.3 (4)	C11—C12—C13—C14	−0.3 (6)
C1—N1—C11—C16	82.2 (4)	C12—C11—C16—C15	−0.1 (6)
C1—C5—C6—C7	177.9 (4)	C12—C13—C14—C15	−0.6 (6)
C1—C5—C10—C9	−178.7 (3)	C13—C14—C15—C16	1.1 (7)
C2—N1—C1—S1	−28.1 (4)	C14—C15—C16—C11	−0.8 (6)
C2—N1—C1—C5	98.7 (4)	C16—C11—C12—C13	0.7 (6)
C2—N1—C11—C12	72.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1[i]	0.98	2.30	3.261 (5)	167

Symmetry code: (i) −x, −y+1, z−1/2.