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3-Chloro-1-methyl-4-[2-(3-phenylallylidene)hydrazinylidene]-3,4-dihydro-1*H*-2λ⁶,1-benzothiazine-2,2-dione

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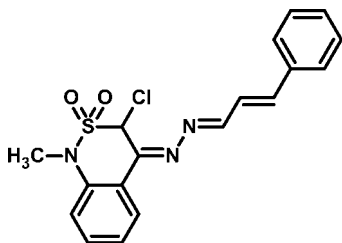
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.067; wR factor = 0.201; data-to-parameter ratio = 13.7.

In the title compound, $\text{C}_{18}\text{H}_{16}\text{ClN}_3\text{O}_2\text{S}$, the dihedral angle between the aromatic rings is $4.81(2)^\circ$ and the alkyl chain takes on an extended conformation [$\text{N}-\text{C}-\text{C}-\text{C} = 179.2(4)^\circ$]. The conformation of the thiazine ring is an envelope, with the S atom displaced by $-0.805(3)$ Å from the mean plane of the other five atoms (r.m.s. deviation = 0.046 Å). The Cl atom is in an axial conformation and is displaced by $1.761(4)$ Å from the thiazine ring plane. In the crystal, inversion dimers linked by pairs of $\text{C}-\text{H}\cdots\text{O}$ interactions generate $R_2^2(20)$ loops and further $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the dimers into (001) sheets. Weak aromatic $\pi-\pi$ stacking interactions [centroid-centroid separations = $3.870(3)$ and $3.883(3)$ Å] are also observed.

Related literature

For the synthesis and biological activity of the title compound and related materials, see: Shafiq *et al.* (2011a). For further synthetic details, see: Shafiq *et al.* (2011b).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{16}\text{ClN}_3\text{O}_2\text{S}$
 $M_r = 373.85$
 Monoclinic, $P2_1/c$
 $a = 7.2262(5)$ Å
 $b = 13.5823(9)$ Å
 $c = 17.9818(12)$ Å
 $\beta = 97.023(4)^\circ$
 $V = 1751.6(2)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.35$ mm⁻¹
 $T = 296$ K
 $0.32 \times 0.20 \times 0.18$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.895$, $T_{\max} = 0.939$
 8051 measured reflections
 3107 independent reflections
 1808 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.201$
 $S = 1.03$
 3107 reflections
 227 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.97$ e Å⁻³
 $\Delta\rho_{\min} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C12}-\text{H12}\cdots\text{O2}^i$	0.93	2.51	3.345 (6)	150
$\text{C15}-\text{H15}\cdots\text{O2}^{ii}$	0.93	2.57	3.464 (6)	161

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

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, 2012); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2381).

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supporting information

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3-Chloro-1-methyl-4-[2-(3-phenylallylidene)hydrazinylidene]-3,4-dihydro-1*H*-2λ⁶,1-benzothiazine-2,2-dione

Muhammad Shafiq, M. Nawaz Tahir, William T. A. Harrison, Islam Ullah Khan and Sidra Shafique

S1. Comment

As part of our ongoing studies of benzothiazine derivatives with potential biactivity (Shafiq *et al.*, 2011*a,b*), we now describe the synthesis and structure of the title compound, (I).

The dihedral angle between the C1–C6 and C13–C18 aromatic rings is 4.81 (2)° and the C9=N2—N3=C10 torsion angle is -178.1 (4)°. The linking alkyl chain takes on an extended conformation [N3—C10—C11—C12 = 179.2 (4)°]. The conformation of the C1/C6/C8/C9/N1/S1 thiazine ring is an envelope, with the S atom displaced by -0.805 (3) Å from the mean plane of the other five atoms (r.m.s. deviation = 0.046 Å). Atom C16 is displaced from the mean plane by 0.343 (6) Å and C11, in an axial site, is displaced by 1.761 (4) Å. Atom C8 is a stereogenic centre (*R* configuration in the arbitrarily-chosen asymmetric unit), but crystal symmetry generates a racemic mixture.

In the crystal, inversion dimers linked by pairs of C—H···O interactions (Table 1) to generate $R_2^2(20)$ loops. Further C—H···O bonds link the dimers into (001) sheets. Weak aromatic π - π stacking interactions between the C1—C6 and C13—C18 benzene rings [centroid-centroid separations = 3.870 (3) and 3.883 (3) Å] are also observed.

S2. Experimental

The Schiff base derivative of (4*Z*)-4-hydrazinylidene-1-methyl-3,4-dihydro-1*H*-2,1-benzothiazine 2,2-dioxide and *trans* cinnamaldehyde was prepared using the methods reported previously (Shafiq *et al.*, 2011*a*). The chlorination of the Schiff base was undertaken using *N*-chloro succinimide and dibenzoylperoxide (Shafiq *et al.*, 2011*b*). The crude product was recrystallized from ethyl acetate solution to obtain yellow blocks of the title compound.

S3. Refinement

The H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined as riding. The methyl group was allowed to rotate, but not to tip, to best fit the electron density. The constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$ was applied.

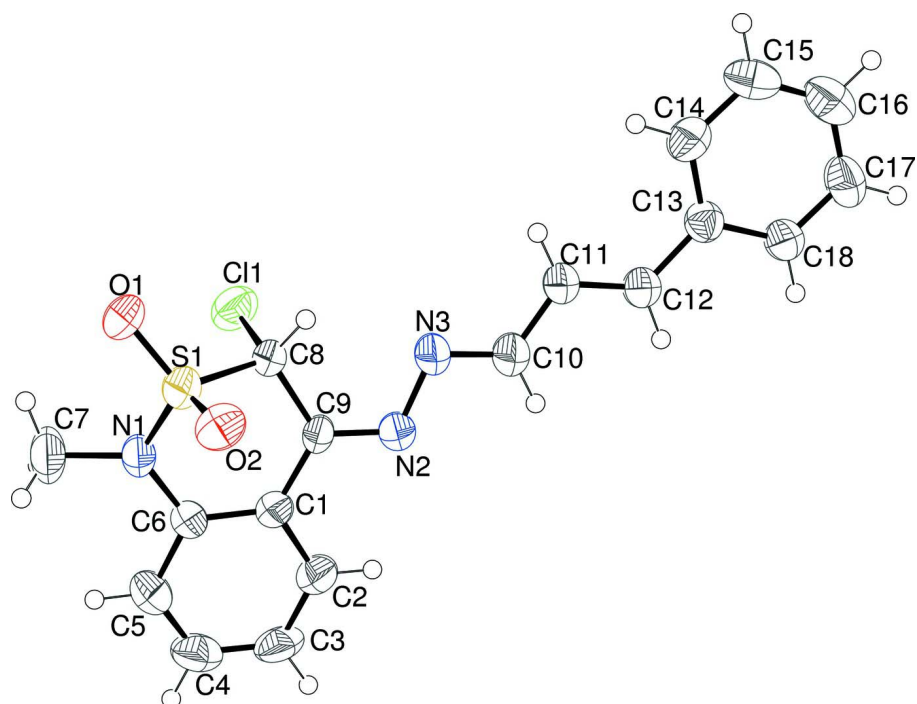


Figure 1

The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

3-Chloro-1-methyl-4-[2-(3-phenylallylidene)hydrazinylidene]-3,4-dihydro-1H-2λ⁶,1-benzothiazine-2,2-dione

Crystal data

$C_{18}H_{16}ClN_3O_2S$

$M_r = 373.85$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 7.2262$ (5) Å

$b = 13.5823$ (9) Å

$c = 17.9818$ (12) Å

$\beta = 97.023$ (4)°

$V = 1751.6$ (2) Å³

$Z = 4$

$F(000) = 776$

$D_x = 1.418$ Mg m⁻³

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

Cell parameters from 305 reflections

$\theta = 3.5$ – 24.5 °

$\mu = 0.35$ mm⁻¹

$T = 296$ K

Rod, yellow

$0.32 \times 0.20 \times 0.18$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)

$T_{\min} = 0.895$, $T_{\max} = 0.939$

8051 measured reflections

3107 independent reflections

1808 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 25.5$ °, $\theta_{\min} = 2.7$ °

$h = -8 \rightarrow 8$

$k = -13 \rightarrow 16$

$l = -21 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.201$
 $S = 1.03$
 3107 reflections
 227 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
 $w = 1/[\sigma^2(F_o^2) + (0.1036P)^2 + 0.2998P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.97 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2953 (5)	0.2779 (3)	0.6118 (2)	0.0406 (11)
C2	0.3170 (6)	0.3399 (4)	0.6745 (3)	0.0526 (12)
H2	0.3146	0.4077	0.6673	0.063*
C3	0.3415 (7)	0.3037 (4)	0.7460 (3)	0.0601 (14)
H3	0.3549	0.3465	0.7867	0.072*
C4	0.3463 (7)	0.2037 (4)	0.7574 (3)	0.0622 (14)
H4	0.3660	0.1791	0.8059	0.075*
C5	0.3225 (7)	0.1399 (4)	0.6983 (3)	0.0584 (13)
H5	0.3231	0.0724	0.7069	0.070*
C6	0.2973 (6)	0.1759 (3)	0.6248 (2)	0.0422 (11)
C7	0.3297 (8)	0.0041 (3)	0.5761 (3)	0.0762 (17)
H7A	0.4520	0.0003	0.6036	0.114*
H7B	0.3302	-0.0271	0.5282	0.114*
H7C	0.2419	-0.0286	0.6036	0.114*
C8	0.2780 (6)	0.2531 (3)	0.4704 (3)	0.0422 (11)
H8	0.2142	0.2856	0.4257	0.051*
C9	0.2729 (5)	0.3201 (3)	0.5368 (2)	0.0381 (10)
C10	0.2243 (6)	0.5395 (3)	0.4480 (3)	0.0507 (12)
H10	0.2233	0.5762	0.4916	0.061*
C11	0.2092 (6)	0.5897 (3)	0.3787 (3)	0.0489 (12)
H11	0.2116	0.5542	0.3345	0.059*
C12	0.1917 (6)	0.6871 (3)	0.3759 (3)	0.0480 (12)
H12	0.1893	0.7181	0.4219	0.058*
C13	0.1756 (6)	0.7522 (3)	0.3107 (3)	0.0450 (11)
C14	0.1646 (7)	0.7194 (4)	0.2366 (3)	0.0563 (13)

H14	0.1665	0.6522	0.2266	0.068*
C15	0.1508 (7)	0.7866 (5)	0.1777 (3)	0.0634 (14)
H15	0.1434	0.7639	0.1287	0.076*
C16	0.1482 (7)	0.8848 (5)	0.1912 (3)	0.0683 (15)
H16	0.1402	0.9291	0.1515	0.082*
C17	0.1573 (7)	0.9191 (4)	0.2634 (3)	0.0638 (14)
H17	0.1536	0.9864	0.2725	0.077*
C18	0.1717 (6)	0.8543 (3)	0.3220 (3)	0.0517 (12)
H18	0.1791	0.8786	0.3706	0.062*
S1	0.15957 (18)	0.14181 (8)	0.48575 (7)	0.0514 (4)
O1	0.1890 (5)	0.0698 (2)	0.42999 (19)	0.0666 (10)
O2	-0.0251 (4)	0.1739 (2)	0.49385 (18)	0.0542 (9)
N1	0.2763 (5)	0.1075 (3)	0.5651 (2)	0.0518 (10)
N2	0.2523 (5)	0.4134 (3)	0.5278 (2)	0.0478 (10)
N3	0.2393 (5)	0.4455 (3)	0.4536 (2)	0.0526 (10)
Cl1	0.51237 (17)	0.22812 (9)	0.45547 (8)	0.0621 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.043 (2)	0.041 (3)	0.039 (3)	0.0041 (18)	0.0078 (19)	-0.002 (2)
C2	0.064 (3)	0.050 (3)	0.044 (3)	0.006 (2)	0.007 (2)	-0.006 (3)
C3	0.071 (3)	0.075 (4)	0.034 (3)	0.009 (3)	0.006 (2)	-0.016 (3)
C4	0.066 (3)	0.082 (4)	0.038 (3)	0.007 (3)	0.007 (2)	0.009 (3)
C5	0.071 (3)	0.054 (3)	0.049 (3)	0.006 (2)	0.004 (2)	0.013 (3)
C6	0.049 (3)	0.040 (3)	0.038 (3)	0.0043 (19)	0.006 (2)	0.004 (2)
C7	0.116 (5)	0.035 (3)	0.074 (4)	0.008 (3)	-0.004 (3)	0.004 (3)
C8	0.058 (3)	0.032 (2)	0.037 (3)	0.0042 (18)	0.009 (2)	-0.001 (2)
C9	0.045 (2)	0.028 (2)	0.041 (3)	0.0045 (17)	0.0049 (19)	-0.003 (2)
C10	0.063 (3)	0.038 (3)	0.051 (3)	0.002 (2)	0.006 (2)	0.000 (2)
C11	0.065 (3)	0.036 (3)	0.047 (3)	0.001 (2)	0.010 (2)	0.002 (2)
C12	0.060 (3)	0.038 (3)	0.046 (3)	-0.003 (2)	0.010 (2)	0.000 (2)
C13	0.046 (3)	0.042 (3)	0.046 (3)	-0.0007 (18)	0.003 (2)	0.000 (2)
C14	0.065 (3)	0.049 (3)	0.055 (4)	-0.001 (2)	0.008 (2)	-0.009 (3)
C15	0.061 (3)	0.088 (4)	0.039 (3)	-0.009 (3)	0.001 (2)	0.002 (3)
C16	0.065 (3)	0.080 (4)	0.061 (4)	-0.002 (3)	0.010 (3)	0.024 (3)
C17	0.072 (3)	0.046 (3)	0.073 (4)	-0.003 (2)	0.011 (3)	0.016 (3)
C18	0.065 (3)	0.042 (3)	0.050 (3)	-0.003 (2)	0.013 (2)	0.003 (2)
S1	0.0683 (9)	0.0383 (7)	0.0475 (8)	-0.0027 (5)	0.0070 (6)	-0.0040 (6)
O1	0.109 (3)	0.0401 (19)	0.052 (2)	-0.0042 (17)	0.0127 (19)	-0.0149 (17)
O2	0.0472 (19)	0.060 (2)	0.055 (2)	-0.0051 (14)	0.0033 (15)	-0.0113 (17)
N1	0.081 (3)	0.031 (2)	0.042 (3)	0.0058 (17)	0.0017 (19)	0.0016 (19)
N2	0.066 (3)	0.038 (2)	0.039 (2)	0.0037 (16)	0.0049 (18)	0.0004 (18)
N3	0.076 (3)	0.035 (2)	0.046 (3)	0.0026 (18)	0.0063 (19)	0.0018 (19)
Cl1	0.0630 (8)	0.0605 (8)	0.0664 (10)	0.0036 (5)	0.0223 (6)	-0.0108 (7)

Geometric parameters (Å, °)

C1—C2	1.401 (6)	C10—C11	1.414 (6)
C1—C6	1.405 (6)	C10—H10	0.9300
C1—C9	1.455 (6)	C11—C12	1.329 (6)
C2—C3	1.368 (7)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.462 (6)
C3—C4	1.373 (7)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.398 (7)
C4—C5	1.365 (7)	C13—C18	1.402 (6)
C4—H4	0.9300	C14—C15	1.393 (7)
C5—C6	1.399 (6)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.357 (7)
C6—N1	1.415 (6)	C15—H15	0.9300
C7—N1	1.463 (6)	C16—C17	1.373 (7)
C7—H7A	0.9600	C16—H16	0.9300
C7—H7B	0.9600	C17—C18	1.366 (6)
C7—H7C	0.9600	C17—H17	0.9300
C8—C9	1.506 (6)	C18—H18	0.9300
C8—S1	1.775 (4)	S1—O2	1.428 (3)
C8—C11	1.780 (4)	S1—O1	1.435 (3)
C8—H8	0.9800	S1—N1	1.634 (4)
C9—N2	1.283 (5)	N2—N3	1.397 (5)
C10—N3	1.284 (5)		
C2—C1—C6	117.4 (4)	C12—C11—C10	120.7 (5)
C2—C1—C9	119.8 (4)	C12—C11—H11	119.7
C6—C1—C9	122.8 (4)	C10—C11—H11	119.7
C3—C2—C1	122.0 (5)	C11—C12—C13	129.1 (5)
C3—C2—H2	119.0	C11—C12—H12	115.4
C1—C2—H2	119.0	C13—C12—H12	115.4
C2—C3—C4	119.5 (5)	C14—C13—C18	117.0 (4)
C2—C3—H3	120.2	C14—C13—C12	124.0 (4)
C4—C3—H3	120.2	C18—C13—C12	119.0 (4)
C5—C4—C3	120.9 (5)	C15—C14—C13	120.4 (5)
C5—C4—H4	119.5	C15—C14—H14	119.8
C3—C4—H4	119.5	C13—C14—H14	119.8
C4—C5—C6	120.2 (5)	C16—C15—C14	120.7 (5)
C4—C5—H5	119.9	C16—C15—H15	119.7
C6—C5—H5	119.9	C14—C15—H15	119.7
C5—C6—C1	120.0 (4)	C15—C16—C17	120.2 (5)
C5—C6—N1	118.5 (4)	C15—C16—H16	119.9
C1—C6—N1	121.5 (4)	C17—C16—H16	119.9
N1—C7—H7A	109.5	C18—C17—C16	120.0 (5)
N1—C7—H7B	109.5	C18—C17—H17	120.0
H7A—C7—H7B	109.5	C16—C17—H17	120.0
N1—C7—H7C	109.5	C17—C18—C13	121.8 (5)
H7A—C7—H7C	109.5	C17—C18—H18	119.1

H7B—C7—H7C	109.5	C13—C18—H18	119.1
C9—C8—S1	109.4 (3)	O2—S1—O1	120.0 (2)
C9—C8—C11	110.5 (3)	O2—S1—N1	112.8 (2)
S1—C8—C11	110.3 (2)	O1—S1—N1	108.1 (2)
C9—C8—H8	108.9	O2—S1—C8	103.3 (2)
S1—C8—H8	108.9	O1—S1—C8	110.9 (2)
C11—C8—H8	108.9	N1—S1—C8	99.9 (2)
N2—C9—C1	120.3 (4)	C6—N1—C7	121.7 (4)
N2—C9—C8	120.7 (4)	C6—N1—S1	118.1 (3)
C1—C9—C8	119.1 (4)	C7—N1—S1	119.4 (3)
N3—C10—C11	123.1 (5)	C9—N2—N3	115.0 (4)
N3—C10—H10	118.5	C10—N3—N2	112.4 (4)
C11—C10—H10	118.5		
C6—C1—C2—C3	0.8 (6)	C14—C15—C16—C17	-0.7 (8)
C9—C1—C2—C3	-178.9 (4)	C15—C16—C17—C18	0.9 (8)
C1—C2—C3—C4	0.4 (7)	C16—C17—C18—C13	-0.7 (7)
C2—C3—C4—C5	-1.5 (7)	C14—C13—C18—C17	0.2 (7)
C3—C4—C5—C6	1.5 (7)	C12—C13—C18—C17	179.9 (4)
C4—C5—C6—C1	-0.4 (7)	C9—C8—S1—O2	60.3 (3)
C4—C5—C6—N1	178.9 (4)	C11—C8—S1—O2	-178.0 (2)
C2—C1—C6—C5	-0.8 (6)	C9—C8—S1—O1	-170.0 (3)
C9—C1—C6—C5	178.9 (4)	C11—C8—S1—O1	-48.2 (3)
C2—C1—C6—N1	180.0 (4)	C9—C8—S1—N1	-56.2 (3)
C9—C1—C6—N1	-0.4 (6)	C11—C8—S1—N1	65.6 (3)
C2—C1—C9—N2	-7.8 (6)	C5—C6—N1—C7	-16.9 (6)
C6—C1—C9—N2	172.6 (4)	C1—C6—N1—C7	162.4 (4)
C2—C1—C9—C8	171.1 (4)	C5—C6—N1—S1	153.4 (3)
C6—C1—C9—C8	-8.5 (6)	C1—C6—N1—S1	-27.4 (5)
S1—C8—C9—N2	-142.1 (3)	O2—S1—N1—C6	-56.8 (4)
C11—C8—C9—N2	96.3 (4)	O1—S1—N1—C6	168.2 (3)
S1—C8—C9—C1	39.1 (5)	C8—S1—N1—C6	52.3 (4)
C11—C8—C9—C1	-82.5 (4)	O2—S1—N1—C7	113.7 (4)
N3—C10—C11—C12	179.2 (4)	O1—S1—N1—C7	-21.3 (4)
C10—C11—C12—C13	179.5 (4)	C8—S1—N1—C7	-137.2 (4)
C11—C12—C13—C14	4.2 (7)	C1—C9—N2—N3	177.7 (3)
C11—C12—C13—C18	-175.5 (5)	C8—C9—N2—N3	-1.2 (5)
C18—C13—C14—C15	0.1 (7)	C11—C10—N3—N2	180.0 (4)
C12—C13—C14—C15	-179.5 (4)	C9—N2—N3—C10	-178.1 (4)
C13—C14—C15—C16	0.1 (7)		

Hydrogen-bond geometry (Å, °)

<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>
C12—H12 \cdots O2 ⁱ	0.93	2.51	3.345 (6)	150
C15—H15 \cdots O2 ⁱⁱ	0.93	2.57	3.464 (6)	161

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