Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-{(*E*)-[(2*Z*)-(3-Chloro-1-methyl-2,2-dioxo-3,4-dihydro-1*H*-2,1-benzothiazin-4-ylidene)hydrazinylidene]methyl}phenol

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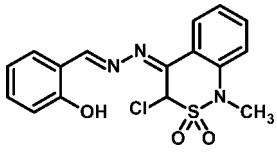
Received 15 December 2011; accepted 28 December 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.073; wR factor = 0.211; data-to-parameter ratio = 18.0.

In the title compound, $C_{16}H_{14}ClN_3O_3S$, the thiazine ring adopts a sofa (half-chair) conformation, with an r.m.s. deviation from the mean plane of 0.23 Å. The S atom and S-bonded C atom exhibit the maximum deviations from the thiazine mean plane [−0.3976 (12) and 0.3179 (14) Å, respectively]. The conformations around the double bonds in the $R_2C{=}N{-}N{=}CHR$ unit are *Z* and *E*. An intramolecular O—H···N hydrogen bond with the hydroxy group as donor generates an *S*(6) ring motif. In the crystal, pairs of weak C—H···O interactions connect the molecules, forming inversion dimers.

Related literature

For benzothiazine compounds, see: Shafiq, Khan *et al.* (2011); Shafiq, Zia-ur-Rehman *et al.* (2011). For related structures, see: Shafiq *et al.* (2011*a*,*b*). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{16}H_{14}ClN_3O_3S$
M_r = 363.81
Monoclinic, $P2_1/c$
a = 7.0973 (5) Å
b = 12.0957 (7) Å
c = 18.7396 (13) Å
β = 96.058 (4)°
V = 1599.75 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 296 K
0.19 × 0.08 × 0.07 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.930, T_{max} = 0.973
15526 measured reflections
3977 independent reflections
2200 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.211
S = 1.03
3977 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*O*···N3	0.82 (7)	1.98 (7)	2.682 (5)	143 (7)
C9—H9···O1^{i}	0.95	2.55	3.394 (5)	148

Symmetry code: (i) $-x, -y+1, -z+1$.

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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the Higher Education Commission of Pakistan for providing a grant for the project to strengthen the Materials Chemistry Laboratory at GC University Lahore, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2407).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Shafiq, M., Khan, I. U., Arshad, M. N. & Siddiqui, W. A. (2011). *Asian J. Chem.* **23**, 2101-2105.
Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011*a*). *Acta Cryst.* E**67**, o2038.
Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011*b*). *Acta Cryst.* E**67**, o2092.
Shafiq, M., Zia-ur-Rehman, M., Khan, I. U., Arshad, M. N. & Khan, S. A. (2011). *J. Chil. Chem. Soc.* **56**, 527–531.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o307 [doi:10.1107/S1600536811055978]

2-{(*E*)-[(2*Z*)-(3-Chloro-1-methyl-2,2-dioxo-3,4-dihydro-1*H*-2,1-benzothiazin-4-ylidene)hydrazinylidene]methyl}phenol

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S1. Comment

We have recently explored the synthesis of different halogenated benzothiazines (Shafiq, Khan, Arshad *et al.*, 2011), and their Schiff bases (Shafiq, Zia-ur-Rehman *et al.*, 2011). The crystal structure of title compound is being reported in order to study the geometry and different interactions in this class of compounds.

The present structure relates with the already published crystal structures of 4-hydrazinylidene-1-methyl-3*H*-2λ^6,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*a*) and 6-bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3*H*-2λ^6,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*b*). The two fused rings in the title compound (Fig. 1) are oriented at dihedral angle of 7.49 (5)° and the thiazine ring adopts the sofa shape with r.m.s. deviation of about 0.23 Å, and with the maximum deviations arising from S1 [-0.3721 (21) Å] and C8 [0.3118 (26) Å] atoms. The intramolecular hydrogen bonding interaction of O—H···N type generates a six membered ring $S_1^1(6)$ (Bernstein *et al.*, 1995). A weak C—H···O type interaction connects the molecules to form centrosymmetric dimers and generates $R_2^2(16)$ ring motifs (Bernstein *et al.*, 1995; Table 1 and Fig. 2).

The phenol ring is oriented at dihedral angle of 8.17 (4) and 15.58 (5)° with respect to the aromatic ring and thiazine ring, and is twisted by 2.07 (3)° with respect to six membered *S*(6) ring motif generated through the intramolecular O—H···N hydrogen bond.

S2. Experimental

For the synthesis of title compound, 4-hydrazinylidene-1- methyl-3*H*-2λ^6,1-benzothiazine-2,2-dione (Shafiq, Khan, Zia-ur-Rehman *et al.*, 2011*a*) was subjected to react with salicylaldehyde according to literature procedure (Shafiq, Zia-ur-Rehman *et al.*, 2011). The product obtained was then halogenated following another method (Shafiq, Khan, Arshad *et al.*, 2011). Suitable crystals were produced by slow evaporation of a dry ethylacetate solution.

S3. Refinement

All C-bonded H-atoms were positioned in idealized geometry, with C—H = 0.95 Å for aromatic CH, C—H = 0.98 Å for the methyl group, and C—H = 1 Å for methine C8, and were refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C) for aromatic groups and C8, and U_{iso}(H) = 1.5U_{eq}(C16) for the methyl group. Hydroxyl H atom H3O was found in a difference map and refined freely, restraining the O—H bond length to 0.82 (7) Å, with U_{iso}(H3O) = 2U_{eq}(O3).

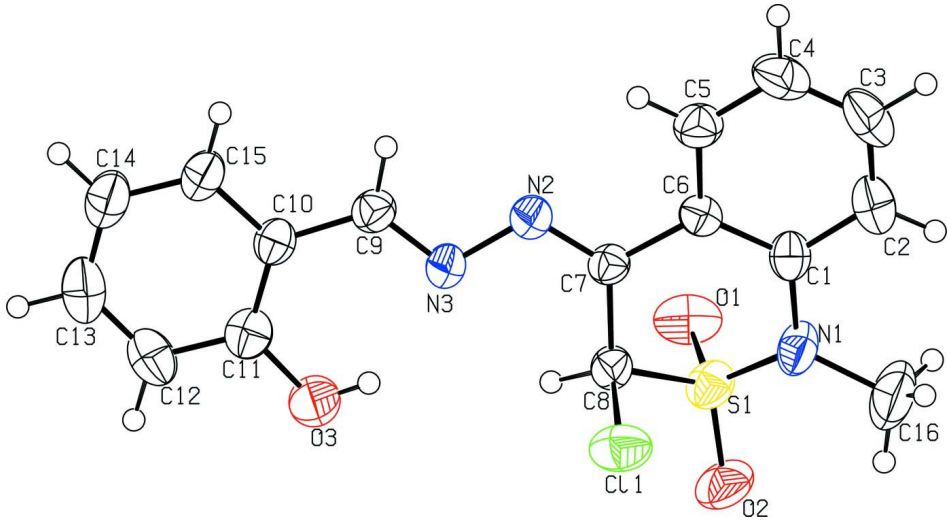

Figure 1

The molecular structure of the title compound showing 50% displacement ellipsoids.

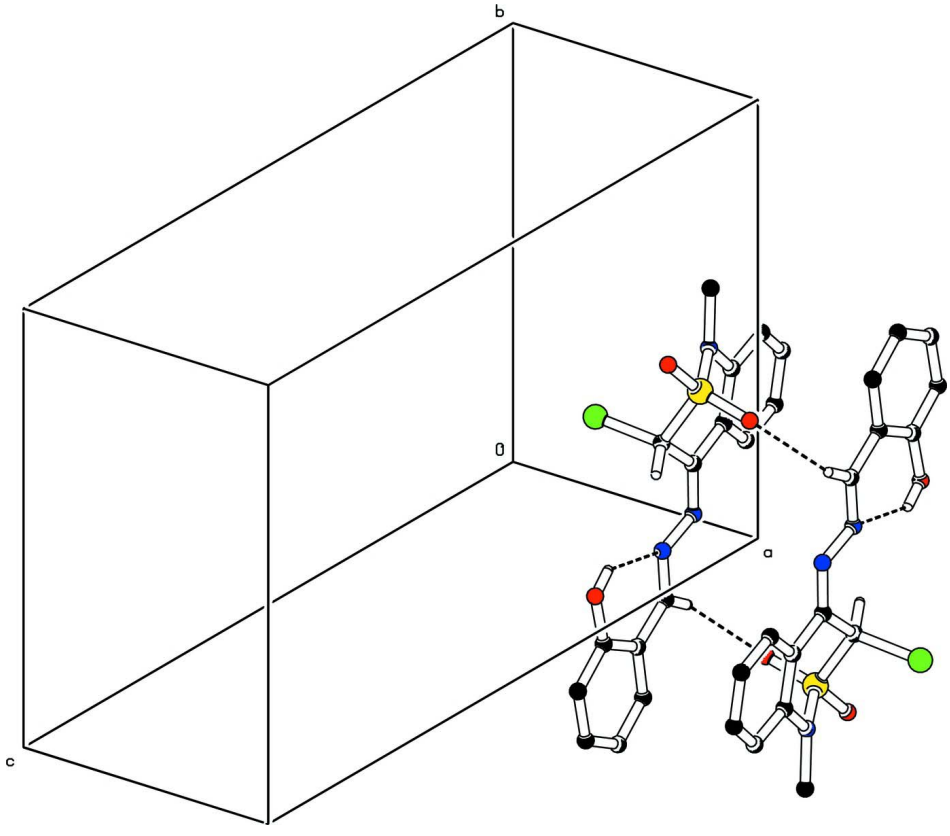

Figure 2

Perspective view which shows the dimers formed through C—H···O hydrogen bonds (dashed lines).

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$b = 12.0957$ (7) Å
$c = 18.7396$ (13) Å
$\beta = 96.058$ (4)°
$V = 1599.75$ (18) Å^3
$Z = 4$
$F(000) = 752$
$D_x = 1.511$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2110 reflections
$\theta = 2.8$–$23.7°$
$\mu = 0.39$ mm^{-1}
$T = 296$ K
Needle, colourless
0.19 × 0.08 × 0.07 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.930$, $T_{max} = 0.973$
15526 measured reflections
3977 independent reflections
2200 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.9°$
$h = -8 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -24 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.211$
$S = 1.03$
3977 reflections
221 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 1.6824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.13$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.51356 (17)	0.73641 (10)	0.42510 (7)	0.0613 (4)
S1	0.16021 (16)	0.83188 (8)	0.46237 (6)	0.0466 (3)
O1	−0.0316 (4)	0.7950 (3)	0.46762 (18)	0.0589 (9)
O2	0.1931 (5)	0.9186 (2)	0.41328 (19)	0.0646 (10)
O3	0.2121 (6)	0.4788 (3)	0.27384 (18)	0.0632 (10)
N1	0.2779 (5)	0.8598 (3)	0.5392 (2)	0.0486 (9)
N2	0.2405 (5)	0.5211 (3)	0.48831 (18)	0.0410 (8)
N3	0.2244 (5)	0.4863 (2)	0.41731 (18)	0.0409 (8)
C1	0.2935 (6)	0.7761 (3)	0.5927 (2)	0.0393 (9)
C2	0.3168 (7)	0.8064 (4)	0.6654 (2)	0.0546 (12)
H2	0.3185	0.8823	0.6784	0.066*
C3	0.3368 (7)	0.7278 (5)	0.7172 (3)	0.0625 (14)

H3	0.3541	0.7496	0.7662	0.075*
C4	0.3327 (7)	0.6172 (4)	0.7003 (2)	0.0576 (12)
H4	0.3462	0.5629	0.7371	0.069*
C5	0.3090 (6)	0.5861 (4)	0.6295 (2)	0.0466 (10)
H5	0.3059	0.5097	0.6178	0.056*
C6	0.2894 (5)	0.6638 (3)	0.5745 (2)	0.0349 (8)
C7	0.2647 (5)	0.6248 (3)	0.4995 (2)	0.0340 (8)
C8	0.2740 (6)	0.7083 (3)	0.4402 (2)	0.0402 (9)
H8	0.2059	0.6776	0.3950	0.048*
C9	0.2063 (6)	0.3806 (3)	0.4143 (2)	0.0399 (9)
H9	0.2041	0.3408	0.4579	0.048*
C10	0.1889 (5)	0.3193 (3)	0.3476 (2)	0.0383 (9)
C11	0.1917 (6)	0.3688 (3)	0.2807 (2)	0.0448 (10)
C12	0.1740 (7)	0.3036 (4)	0.2194 (3)	0.0570 (12)
H12	0.1764	0.3368	0.1736	0.068*
C13	0.1532 (7)	0.1921 (4)	0.2249 (3)	0.0628 (14)
H13	0.1388	0.1487	0.1824	0.075*
C14	0.1526 (7)	0.1407 (4)	0.2903 (3)	0.0568 (12)
H14	0.1393	0.0628	0.2932	0.068*
C15	0.1715 (6)	0.2043 (3)	0.3513 (3)	0.0464 (10)
H15	0.1728	0.1695	0.3968	0.056*
C16	0.3125 (10)	0.9768 (4)	0.5597 (3)	0.0839 (18)
H16A	0.2108	1.0030	0.5869	0.126*
H16B	0.3153	1.0217	0.5163	0.126*
H16C	0.4343	0.9831	0.5893	0.126*
H3O	0.235 (11)	0.509 (6)	0.313 (4)	0.126*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0542 (7)	0.0619 (7)	0.0709 (9)	0.0012 (6)	0.0213 (6)	0.0147 (6)
S1	0.0503 (7)	0.0366 (5)	0.0514 (7)	0.0043 (5)	−0.0005 (5)	0.0050 (5)
O1	0.0359 (17)	0.073 (2)	0.066 (2)	0.0084 (15)	−0.0010 (14)	0.0259 (17)
O2	0.086 (3)	0.0398 (17)	0.066 (2)	−0.0017 (16)	−0.0010 (18)	0.0182 (15)
O3	0.094 (3)	0.0417 (18)	0.054 (2)	0.0080 (17)	0.0063 (19)	0.0097 (15)
N1	0.060 (2)	0.0312 (17)	0.052 (2)	0.0033 (16)	−0.0057 (17)	−0.0064 (15)
N2	0.049 (2)	0.0353 (17)	0.038 (2)	−0.0009 (15)	0.0044 (15)	−0.0005 (14)
N3	0.052 (2)	0.0315 (16)	0.040 (2)	−0.0002 (14)	0.0060 (15)	−0.0033 (14)
C1	0.035 (2)	0.041 (2)	0.041 (2)	0.0017 (17)	−0.0009 (17)	−0.0064 (18)
C2	0.055 (3)	0.062 (3)	0.045 (3)	0.001 (2)	0.001 (2)	−0.016 (2)
C3	0.058 (3)	0.095 (4)	0.034 (3)	−0.005 (3)	0.004 (2)	−0.015 (3)
C4	0.061 (3)	0.075 (3)	0.037 (3)	−0.004 (2)	0.004 (2)	0.011 (2)
C5	0.051 (3)	0.046 (2)	0.042 (3)	−0.0043 (19)	0.0007 (19)	0.0059 (19)
C6	0.032 (2)	0.040 (2)	0.033 (2)	−0.0003 (16)	0.0024 (15)	0.0014 (17)
C7	0.036 (2)	0.0306 (18)	0.035 (2)	0.0025 (15)	0.0018 (16)	0.0031 (16)
C8	0.051 (2)	0.0322 (19)	0.037 (2)	0.0031 (17)	0.0035 (18)	0.0001 (17)
C9	0.042 (2)	0.035 (2)	0.043 (2)	0.0007 (17)	0.0047 (18)	0.0022 (17)
C10	0.037 (2)	0.0342 (19)	0.043 (2)	0.0021 (16)	0.0013 (17)	−0.0020 (17)

C11	0.042 (2)	0.042 (2)	0.050 (3)	0.0069 (18)	−0.0001 (19)	0.0010 (19)
C12	0.061 (3)	0.069 (3)	0.040 (3)	0.007 (2)	0.000 (2)	−0.006 (2)
C13	0.059 (3)	0.063 (3)	0.066 (3)	0.003 (2)	0.004 (2)	−0.026 (3)
C14	0.056 (3)	0.043 (2)	0.072 (3)	−0.005 (2)	0.011 (2)	−0.015 (2)
C15	0.046 (3)	0.035 (2)	0.059 (3)	−0.0032 (18)	0.007 (2)	−0.007 (2)
C16	0.123 (5)	0.040 (3)	0.086 (4)	−0.004 (3)	−0.005 (4)	−0.016 (3)

Geometric parameters (Å, º)

Cl1—C8	1.786 (4)	C5—C6	1.391 (5)
S1—O2	1.430 (3)	C5—H5	0.9500
S1—O1	1.445 (3)	C6—C7	1.475 (5)
S1—N1	1.623 (4)	C7—C8	1.509 (5)
S1—C8	1.770 (4)	C8—H8	1.0000
O3—C11	1.346 (5)	C9—C10	1.447 (5)
O3—H3O	0.82 (7)	C9—H9	0.9500
N1—C1	1.420 (5)	C10—C11	1.391 (6)
N1—C16	1.479 (6)	C10—C15	1.399 (5)
N2—C7	1.280 (5)	C11—C12	1.388 (6)
N2—N3	1.389 (5)	C12—C13	1.362 (7)
N3—C9	1.286 (5)	C12—H12	0.9500
C1—C6	1.399 (5)	C13—C14	1.374 (7)
C1—C2	1.405 (6)	C13—H13	0.9500
C2—C3	1.355 (7)	C14—C15	1.372 (6)
C2—H2	0.9500	C14—H14	0.9500
C3—C4	1.375 (7)	C15—H15	0.9500
C3—H3	0.9500	C16—H16A	0.9800
C4—C5	1.371 (6)	C16—H16B	0.9800
C4—H4	0.9500	C16—H16C	0.9800
O2—S1—O1	119.2 (2)	C7—C8—S1	109.6 (3)
O2—S1—N1	108.3 (2)	C7—C8—Cl1	111.1 (3)
O1—S1—N1	113.8 (2)	S1—C8—Cl1	110.0 (2)
O2—S1—C8	111.0 (2)	C7—C8—H8	108.7
O1—S1—C8	102.2 (2)	S1—C8—H8	108.7
N1—S1—C8	100.35 (19)	Cl1—C8—H8	108.7
C11—O3—H3O	111 (5)	N3—C9—C10	123.1 (4)
C1—N1—C16	120.1 (4)	N3—C9—H9	118.4
C1—N1—S1	118.1 (3)	C10—C9—H9	118.4
C16—N1—S1	119.0 (3)	C11—C10—C15	118.8 (4)
C7—N2—N3	116.8 (3)	C11—C10—C9	123.3 (4)
C9—N3—N2	110.0 (3)	C15—C10—C9	117.9 (4)
C6—C1—C2	119.1 (4)	O3—C11—C12	118.9 (4)
C6—C1—N1	121.5 (3)	O3—C11—C10	121.6 (4)
C2—C1—N1	119.4 (4)	C12—C11—C10	119.5 (4)
C3—C2—C1	120.3 (4)	C13—C12—C11	120.1 (5)
C3—C2—H2	119.8	C13—C12—H12	119.9
C1—C2—H2	119.8	C11—C12—H12	119.9

C2—C3—C4	121.3 (4)	C12—C13—C14	121.7 (5)
C2—C3—H3	119.4	C12—C13—H13	119.2
C4—C3—H3	119.4	C14—C13—H13	119.2
C5—C4—C3	119.1 (4)	C15—C14—C13	118.7 (4)
C5—C4—H4	120.4	C15—C14—H14	120.6
C3—C4—H4	120.4	C13—C14—H14	120.6
C4—C5—C6	121.6 (4)	C14—C15—C10	121.2 (4)
C4—C5—H5	119.2	C14—C15—H15	119.4
C6—C5—H5	119.2	C10—C15—H15	119.4
C5—C6—C1	118.5 (4)	N1—C16—H16A	109.5
C5—C6—C7	118.8 (3)	N1—C16—H16B	109.5
C1—C6—C7	122.7 (3)	H16A—C16—H16B	109.5
N2—C7—C6	118.1 (3)	N1—C16—H16C	109.5
N2—C7—C8	123.4 (3)	H16A—C16—H16C	109.5
C6—C7—C8	118.5 (3)	H16B—C16—H16C	109.5

O2—S1—N1—C1	−169.2 (3)	C5—C6—C7—C8	−170.6 (4)
O1—S1—N1—C1	55.7 (4)	C1—C6—C7—C8	9.6 (6)
C8—S1—N1—C1	−52.7 (3)	N2—C7—C8—S1	142.6 (3)
O2—S1—N1—C16	29.7 (5)	C6—C7—C8—S1	−39.0 (4)
O1—S1—N1—C16	−105.4 (4)	N2—C7—C8—Cl1	−95.6 (4)
C8—S1—N1—C16	146.1 (4)	C6—C7—C8—Cl1	82.8 (4)
C7—N2—N3—C9	178.1 (4)	O2—S1—C8—C7	170.5 (3)
C16—N1—C1—C6	−170.4 (4)	O1—S1—C8—C7	−61.3 (3)
S1—N1—C1—C6	28.6 (5)	N1—S1—C8—C7	56.1 (3)
C16—N1—C1—C2	8.4 (6)	O2—S1—C8—Cl1	48.0 (3)
S1—N1—C1—C2	−152.5 (3)	O1—S1—C8—Cl1	176.2 (2)
C6—C1—C2—C3	0.6 (7)	N1—S1—C8—Cl1	−66.4 (2)
N1—C1—C2—C3	−178.3 (4)	N2—N3—C9—C10	−179.2 (3)
C1—C2—C3—C4	−0.8 (8)	N3—C9—C10—C11	0.5 (6)
C2—C3—C4—C5	0.4 (8)	N3—C9—C10—C15	179.5 (4)
C3—C4—C5—C6	0.1 (7)	C15—C10—C11—O3	−178.6 (4)
C4—C5—C6—C1	−0.3 (6)	C9—C10—C11—O3	0.4 (6)
C4—C5—C6—C7	179.9 (4)	C15—C10—C11—C12	1.0 (6)
C2—C1—C6—C5	−0.1 (6)	C9—C10—C11—C12	−180.0 (4)
N1—C1—C6—C5	178.8 (4)	O3—C11—C12—C13	180.0 (4)
C2—C1—C6—C7	179.7 (4)	C10—C11—C12—C13	0.3 (7)
N1—C1—C6—C7	−1.4 (6)	C11—C12—C13—C14	−1.2 (8)
N3—N2—C7—C6	−177.7 (3)	C12—C13—C14—C15	0.7 (8)
N3—N2—C7—C8	0.7 (6)	C13—C14—C15—C10	0.8 (7)
C5—C6—C7—N2	7.9 (5)	C11—C10—C15—C14	−1.6 (6)
C1—C6—C7—N2	−171.9 (4)	C9—C10—C15—C14	179.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···N3	0.82 (7)	1.98 (7)	2.682 (5)	143 (7)

C9—H9···O1^{i}	0.95	2.55	3.394 (5)	148

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.