

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-Ethyl-4-[1-(1-phenylethylidene)-hydrazin-2-ylidene]-3,4-dihydro-1H-2λ⁶,1-benzothiazine-2,2-dione

Muhammad Shafiq,^{a*} Islam Ullah Khan,^b
 Muhammad Nadeem Arshad,^c Iftikhar Hussain Bukhari^a
 and Ejaz^b

^aDepartment of Chemistry, Government College University, Faisalabad 38040, Pakistan, ^bMaterials Chemistry Laboratory, Department of Chemistry, GC University, Lahore 54000, Pakistan, and ^cDepartment of Chemistry, University of Gujrat, Gujrat 50781, Pakistan

Correspondence e-mail: hafizshafique@hotmail.com

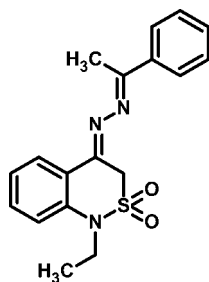
Received 13 May 2012; accepted 19 May 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.046; wR factor = 0.151; data-to-parameter ratio = 18.8.

In the title compound, $\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$, the thiazine ring adopts an envelope conformation, with the S atom displaced by 0.732 (1) Å from the other atoms of the ring. The phenyl ring is oriented at a dihedral angle of 79.33 (7)° with respect to the fused benzene ring. The conformations about the two double bonds in the $\text{R}_2\text{C}=\text{N}-\text{N}=\text{C}(\text{CH}_3)\text{Ar}$ grouping are *Z* and *E*, respectively. In the crystal, inversion dimers linked by pairs of $\text{C}-\text{H}\cdots\text{O}$ interactions generate $R_2^2(8)$ and $R_2^2(12)$ loops, as parts of infinite chains along the *a*-axis direction.

Related literature

For related structures and further synthetic details, see: Shafiq *et al.* (2011*a,b*). For ring puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$
 $M_r = 341.42$
 Monoclinic, $P2_1/n$
 $a = 9.7278$ (3) Å
 $b = 12.4327$ (3) Å
 $c = 14.2607$ (4) Å
 $\beta = 100.725$ (1)°
 $V = 1694.60$ (8) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹
 $T = 296$ K
 $0.41 \times 0.08 \times 0.06$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.920$, $T_{\max} = 0.988$
 16049 measured reflections
 4129 independent reflections
 2887 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.151$
 $S = 1.00$
 4127 reflections
 219 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C8}-\text{H8A}\cdots\text{O1}^{\text{i}}$	0.97	2.43	3.390 (2)	170
$\text{C16}-\text{H16B}\cdots\text{O2}^{\text{ii}}$	0.97	2.52	3.481 (2)	171

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

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

MS acknowledges the Higher Education Commission of Pakistan for supporting PhD studies and for the provision of a grant 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: HB6798).

References

- Bruker (2007). SADABS, APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011*a*). *Acta Cryst.* **E67**, o2038.
 Shafiq, M., Khan, I. U., Zia-ur-Rehman, M., Arshad, M. N. & Asiri, A. M. (2011*b*). *Acta Cryst.* **E67**, o2092.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2012). E68, o1927 [doi:10.1107/S1600536812022982]

1-Ethyl-4-[1-(1-phenylethylidene)hydrazin-2-ylidene]-3,4-dihydro-1*H*-2λ⁶,1-benzothiazine-2,2-dione

Muhammad Shafiq, Islam Ullah Khan, Muhammad Nadeem Arshad, Iftikhar Hussain Bukhari and Ejaz

S1. Comment

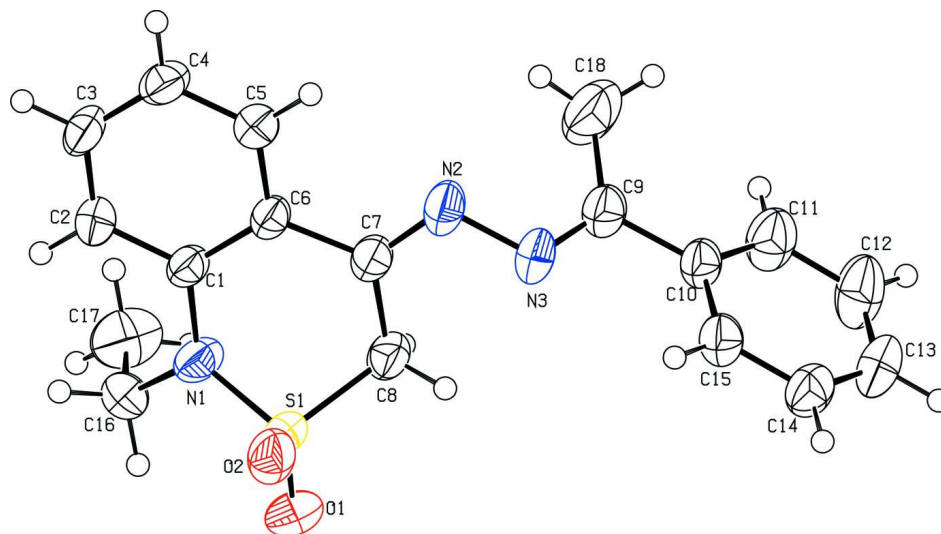
As part of our ongoing studies of benzothiazines, we now describe the title compound, which is related to 4-hydrazinylidene-1-ethyl-3*H*-2λ⁶,1-benzothiazine-2,2-dione and 6-bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3*H*-2λ⁶,1-benzothiazine-2,2-dione. The aromatic and thiazine rings are oriented at dihedral angle of 10.31 (9)° and thiazine ring adopted sofa shape with r. m. s. deviation of about 0.2213 (12)° with the maximum deviation of from the S1 (0.3686 (10)Å) & N1 (0.2640 (11)Å). Thiazine ring shows total ring puckering amplitude QT = 0.5430 Å with (θ) = 55.02 ° (π) = 358.2638 ° (Cremer & Pople, 1975). Both the oxygen atoms of SO₂ group are involved in accepting C—H···O type weak intermolecular hydrogen bonding interaction and produce two ring motifs represented as $R_2^2(8)$ & $R_2^2(12)$ (Table. 1, Fig. 2).

S2. Experimental

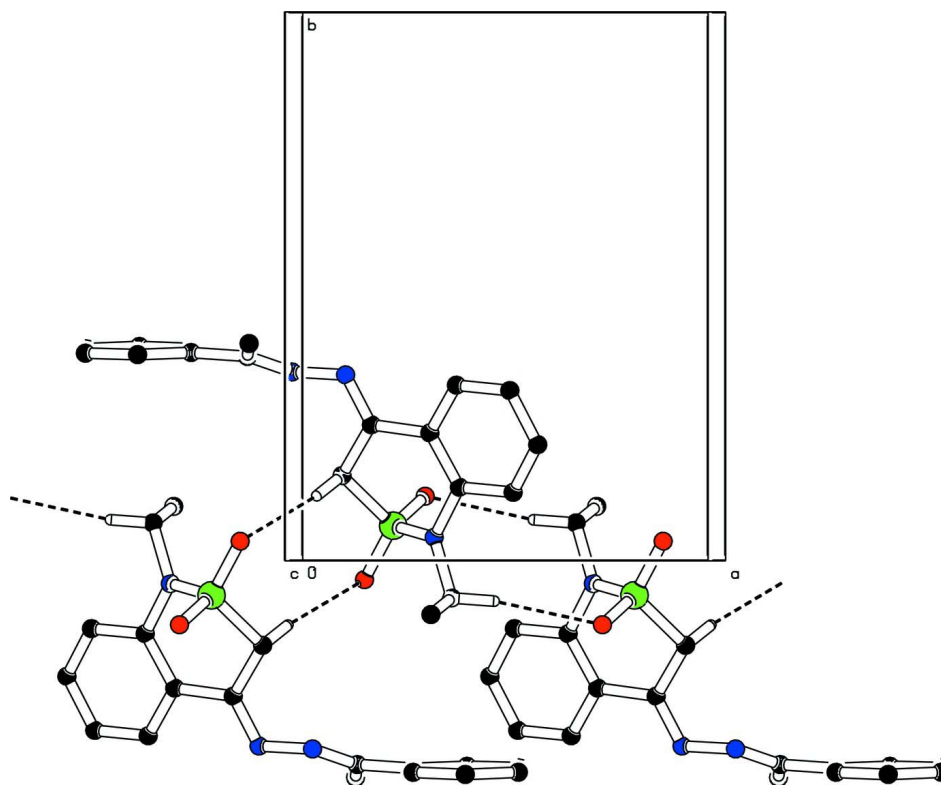
4-Hydrazinylidene-1- methyl-3*H*-2λ⁶,1-benzothiazine-2,2-dione (Shafiq *et al.*, 2011*a*) was subjected to react with acetophenone according to literature procedure (Shafiq *et al.*, 2011*b*). The product obtained was then recrystallized in ethylacetate under slow evaporation to obtain suitable crystal for diffraction studies.

S3. Refinement

All the C—H and H-atoms were positioned with idealized geometry with C—H = 0.93 Å for aromatic, C—H = 0.96 Å for methyl group & C—H = 0.97 Å for methylene and were refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic & methylene and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl carbon atoms. The two reflections (0 0 2) & (0 1 1) were omitted in final refinement.

**Figure 1**

The molecular structure of (I) with 50% displacement ellipsoids.

**Figure 2**

Unit cell packing shows the dimers formed through C—H...O hydrogen bonds, drawn using dashed lines.

1-Ethyl-4-[1-(1-phenylethylidene)hydrazin-2-ylidene]-3,4-dihydro-1*H*-2λ⁶,1-benzothiazine-2,2-dione

Crystal data

C₁₈H₁₉N₃O₂S $M_r = 341.42$ Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

 $a = 9.7278$ (3) Å $b = 12.4327$ (3) Å $c = 14.2607$ (4) Å $\beta = 100.725$ (1)° $V = 1694.60$ (8) Å³ $Z = 4$ $F(000) = 720$ $D_x = 1.338$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4849 reflections

 $\theta = 2.4$ – 26.1 ° $\mu = 0.21$ mm⁻¹ $T = 296$ K

Needle, colorless

 $0.41 \times 0.08 \times 0.06$ 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)

 $T_{\min} = 0.920$, $T_{\max} = 0.988$

16049 measured reflections

4129 independent reflections

2887 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.035$ $\theta_{\text{max}} = 28.3$ °, $\theta_{\text{min}} = 2.2$ ° $h = -12 \rightarrow 12$ $k = -16 \rightarrow 16$ $l = -19 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.151$ $S = 1.00$

4127 reflections

219 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

 $w = 1/[\sigma^2(F_o^2) + (0.0895P)^2 + 0.2125P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.002$ $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Special details

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 (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.78767 (5)	0.93644 (4)	1.05780 (3)	0.04426 (17)
O1	0.85670 (16)	1.03503 (13)	1.08838 (12)	0.0650 (4)
O2	0.71460 (14)	0.88277 (12)	1.12183 (10)	0.0557 (4)
N1	0.68626 (18)	0.95785 (12)	0.95522 (11)	0.0477 (4)

N2	0.89644 (17)	0.66151 (14)	0.96946 (13)	0.0556 (4)
N3	1.02548 (17)	0.65607 (14)	1.03083 (13)	0.0558 (5)
C1	0.62452 (18)	0.86638 (14)	0.90335 (12)	0.0367 (4)
C2	0.49509 (19)	0.87561 (16)	0.84347 (14)	0.0458 (5)
H2	0.4487	0.9414	0.8380	0.055*
C3	0.43489 (19)	0.78866 (17)	0.79221 (14)	0.0496 (5)
H3	0.3487	0.7963	0.7518	0.059*
C4	0.50112 (19)	0.69015 (17)	0.80018 (14)	0.0477 (5)
H4	0.4594	0.6311	0.7662	0.057*
C5	0.62979 (19)	0.68026 (15)	0.85904 (13)	0.0428 (4)
H5	0.6744	0.6138	0.8645	0.051*
C6	0.69472 (16)	0.76729 (14)	0.91056 (12)	0.0355 (4)
C7	0.83541 (17)	0.75244 (15)	0.96944 (13)	0.0401 (4)
C8	0.90722 (18)	0.84518 (16)	1.02506 (14)	0.0473 (5)
H8A	0.9653	0.8820	0.9869	0.057*
H8B	0.9677	0.8183	1.0821	0.057*
C9	1.1295 (2)	0.62777 (15)	0.99497 (15)	0.0497 (5)
C10	1.26558 (19)	0.62074 (14)	1.06248 (13)	0.0428 (4)
C11	1.3907 (2)	0.6245 (2)	1.03087 (17)	0.0634 (6)
H11	1.3910	0.6287	0.9658	0.076*
C12	1.5168 (2)	0.6219 (2)	1.09532 (19)	0.0724 (7)
H12	1.6007	0.6258	1.0731	0.087*
C13	1.5185 (2)	0.61366 (18)	1.19091 (17)	0.0589 (6)
H13	1.6030	0.6108	1.2338	0.071*
C14	1.3945 (2)	0.60965 (17)	1.22303 (15)	0.0534 (5)
H14	1.3951	0.6043	1.2882	0.064*
C15	1.2685 (2)	0.61348 (15)	1.15988 (14)	0.0471 (5)
H15	1.1851	0.6112	1.1828	0.057*
C16	0.6440 (2)	1.06836 (15)	0.92463 (15)	0.0509 (5)
H16A	0.6842	1.1183	0.9745	0.061*
H16B	0.5430	1.0742	0.9159	0.061*
C17	0.6891 (3)	1.0986 (2)	0.83489 (19)	0.0788 (8)
H17A	0.7893	1.0963	0.8440	0.118*
H17B	0.6572	1.1701	0.8170	0.118*
H17C	0.6500	1.0492	0.7854	0.118*
C18	1.1213 (3)	0.6043 (3)	0.89159 (19)	0.0970 (10)
H18A	1.0284	0.5811	0.8643	0.146*
H18B	1.1868	0.5485	0.8844	0.146*
H18C	1.1436	0.6681	0.8596	0.146*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0375 (3)	0.0554 (3)	0.0365 (3)	0.00157 (19)	-0.00216 (19)	-0.0074 (2)
O1	0.0602 (9)	0.0675 (10)	0.0606 (10)	-0.0076 (7)	-0.0063 (8)	-0.0235 (8)
O2	0.0478 (8)	0.0793 (10)	0.0402 (8)	0.0117 (7)	0.0085 (6)	0.0057 (7)
N1	0.0578 (10)	0.0388 (8)	0.0392 (9)	0.0005 (7)	-0.0099 (7)	0.0001 (7)
N2	0.0431 (9)	0.0559 (10)	0.0599 (11)	0.0109 (7)	-0.0106 (8)	0.0007 (9)

N3	0.0418 (9)	0.0636 (11)	0.0548 (11)	0.0136 (8)	-0.0097 (8)	0.0023 (9)
C1	0.0347 (9)	0.0442 (10)	0.0292 (8)	0.0000 (7)	0.0009 (7)	-0.0002 (7)
C2	0.0389 (10)	0.0519 (11)	0.0433 (10)	0.0099 (8)	-0.0009 (8)	0.0002 (9)
C3	0.0335 (9)	0.0670 (13)	0.0425 (11)	0.0018 (8)	-0.0077 (8)	-0.0021 (10)
C4	0.0447 (10)	0.0531 (11)	0.0416 (11)	-0.0072 (8)	-0.0021 (8)	-0.0084 (9)
C5	0.0426 (9)	0.0443 (10)	0.0396 (10)	0.0031 (7)	0.0023 (8)	-0.0025 (8)
C6	0.0307 (8)	0.0441 (10)	0.0300 (8)	0.0010 (7)	0.0014 (6)	0.0022 (7)
C7	0.0332 (9)	0.0498 (10)	0.0358 (9)	0.0016 (7)	0.0027 (7)	0.0014 (8)
C8	0.0306 (9)	0.0653 (12)	0.0437 (11)	0.0009 (8)	0.0010 (8)	-0.0070 (9)
C9	0.0460 (11)	0.0508 (11)	0.0484 (12)	0.0076 (8)	-0.0011 (9)	0.0052 (9)
C10	0.0396 (10)	0.0426 (10)	0.0435 (10)	0.0069 (7)	0.0009 (8)	0.0049 (8)
C11	0.0523 (13)	0.0906 (17)	0.0473 (12)	0.0097 (11)	0.0093 (10)	0.0146 (12)
C12	0.0398 (11)	0.1026 (19)	0.0750 (17)	0.0039 (11)	0.0114 (11)	0.0222 (14)
C13	0.0417 (11)	0.0669 (14)	0.0612 (14)	-0.0007 (9)	-0.0082 (10)	0.0135 (11)
C14	0.0525 (12)	0.0610 (12)	0.0429 (11)	0.0054 (9)	-0.0007 (9)	0.0061 (10)
C15	0.0419 (10)	0.0497 (11)	0.0487 (11)	0.0068 (8)	0.0057 (9)	0.0053 (9)
C16	0.0536 (12)	0.0411 (10)	0.0550 (12)	0.0094 (8)	0.0020 (10)	-0.0072 (9)
C17	0.111 (2)	0.0568 (14)	0.0637 (15)	-0.0098 (14)	0.0021 (15)	0.0094 (12)
C18	0.0702 (17)	0.163 (3)	0.0505 (15)	0.0186 (19)	-0.0083 (13)	-0.0103 (18)

Geometric parameters (Å, °)

S1—O2	1.4232 (15)	C9—C10	1.487 (3)
S1—O1	1.4264 (15)	C9—C18	1.490 (3)
S1—N1	1.6270 (16)	C10—C11	1.376 (3)
S1—C8	1.7493 (19)	C10—C15	1.387 (3)
N1—C1	1.427 (2)	C11—C12	1.390 (3)
N1—C16	1.477 (2)	C11—H11	0.9300
N2—C7	1.277 (2)	C12—C13	1.364 (3)
N2—N3	1.392 (2)	C12—H12	0.9300
N3—C9	1.266 (3)	C13—C14	1.368 (3)
C1—C2	1.388 (2)	C13—H13	0.9300
C1—C6	1.403 (2)	C14—C15	1.380 (3)
C2—C3	1.373 (3)	C14—H14	0.9300
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.379 (3)	C16—C17	1.477 (3)
C3—H3	0.9300	C16—H16A	0.9700
C4—C5	1.377 (2)	C16—H16B	0.9700
C4—H4	0.9300	C17—H17A	0.9600
C5—C6	1.392 (3)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—C7	1.478 (2)	C18—H18A	0.9600
C7—C8	1.497 (3)	C18—H18B	0.9600
C8—H8A	0.9700	C18—H18C	0.9600
C8—H8B	0.9700		
O2—S1—O1	118.02 (10)	N3—C9—C18	123.7 (2)
O2—S1—N1	111.22 (9)	C10—C9—C18	120.4 (2)

O1—S1—N1	107.84 (9)	C11—C10—C15	118.41 (18)
O2—S1—C8	107.66 (9)	C11—C10—C9	121.41 (19)
O1—S1—C8	109.90 (9)	C15—C10—C9	120.15 (18)
N1—S1—C8	100.84 (9)	C10—C11—C12	120.6 (2)
C1—N1—C16	121.41 (15)	C10—C11—H11	119.7
C1—N1—S1	117.52 (12)	C12—C11—H11	119.7
C16—N1—S1	120.46 (13)	C13—C12—C11	120.5 (2)
C7—N2—N3	114.08 (16)	C13—C12—H12	119.7
C9—N3—N2	117.05 (18)	C11—C12—H12	119.7
C2—C1—C6	119.40 (16)	C12—C13—C14	119.3 (2)
C2—C1—N1	119.94 (16)	C12—C13—H13	120.3
C6—C1—N1	120.64 (15)	C14—C13—H13	120.3
C3—C2—C1	120.69 (17)	C13—C14—C15	120.7 (2)
C3—C2—H2	119.7	C13—C14—H14	119.6
C1—C2—H2	119.7	C15—C14—H14	119.6
C2—C3—C4	120.59 (17)	C14—C15—C10	120.42 (19)
C2—C3—H3	119.7	C14—C15—H15	119.8
C4—C3—H3	119.7	C10—C15—H15	119.8
C5—C4—C3	119.17 (17)	N1—C16—C17	112.46 (18)
C5—C4—H4	120.4	N1—C16—H16A	109.1
C3—C4—H4	120.4	C17—C16—H16A	109.1
C4—C5—C6	121.62 (17)	N1—C16—H16B	109.1
C4—C5—H5	119.2	C17—C16—H16B	109.1
C6—C5—H5	119.2	H16A—C16—H16B	107.8
C5—C6—C1	118.50 (15)	C16—C17—H17A	109.5
C5—C6—C7	118.95 (15)	C16—C17—H17B	109.5
C1—C6—C7	122.54 (15)	H17A—C17—H17B	109.5
N2—C7—C6	119.48 (16)	C16—C17—H17C	109.5
N2—C7—C8	120.71 (16)	H17A—C17—H17C	109.5
C6—C7—C8	119.76 (15)	H17B—C17—H17C	109.5
C7—C8—S1	111.91 (12)	C9—C18—H18A	109.5
C7—C8—H8A	109.2	C9—C18—H18B	109.5
S1—C8—H8A	109.2	H18A—C18—H18B	109.5
C7—C8—H8B	109.2	C9—C18—H18C	109.5
S1—C8—H8B	109.2	H18A—C18—H18C	109.5
H8A—C8—H8B	107.9	H18B—C18—H18C	109.5
N3—C9—C10	115.90 (18)		
O2—S1—N1—C1	-59.42 (16)	C1—C6—C7—N2	-176.73 (18)
O1—S1—N1—C1	169.72 (14)	C5—C6—C7—C8	179.76 (17)
C8—S1—N1—C1	54.52 (16)	C1—C6—C7—C8	0.7 (3)
O2—S1—N1—C16	111.72 (17)	N2—C7—C8—S1	-153.81 (16)
O1—S1—N1—C16	-19.14 (19)	C6—C7—C8—S1	28.8 (2)
C8—S1—N1—C16	-134.34 (16)	O2—S1—C8—C7	64.98 (16)
C7—N2—N3—C9	-125.1 (2)	O1—S1—C8—C7	-165.27 (14)
C16—N1—C1—C2	-21.2 (3)	N1—S1—C8—C7	-51.62 (16)
S1—N1—C1—C2	149.88 (15)	N2—N3—C9—C10	-178.94 (16)
C16—N1—C1—C6	157.43 (18)	N2—N3—C9—C18	2.2 (3)

S1—N1—C1—C6	-31.5 (2)	N3—C9—C10—C11	-159.4 (2)
C6—C1—C2—C3	0.7 (3)	C18—C9—C10—C11	19.5 (3)
N1—C1—C2—C3	179.27 (18)	N3—C9—C10—C15	18.7 (3)
C1—C2—C3—C4	0.8 (3)	C18—C9—C10—C15	-162.4 (2)
C2—C3—C4—C5	-1.1 (3)	C15—C10—C11—C12	-0.5 (3)
C3—C4—C5—C6	-0.1 (3)	C9—C10—C11—C12	177.6 (2)
C4—C5—C6—C1	1.5 (3)	C10—C11—C12—C13	1.2 (4)
C4—C5—C6—C7	-177.54 (17)	C11—C12—C13—C14	-1.0 (4)
C2—C1—C6—C5	-1.8 (3)	C12—C13—C14—C15	0.2 (3)
N1—C1—C6—C5	179.60 (17)	C13—C14—C15—C10	0.4 (3)
C2—C1—C6—C7	177.25 (16)	C11—C10—C15—C14	-0.3 (3)
N1—C1—C6—C7	-1.4 (3)	C9—C10—C15—C14	-178.37 (18)
N3—N2—C7—C6	-177.29 (16)	C1—N1—C16—C17	-69.1 (3)
N3—N2—C7—C8	5.3 (3)	S1—N1—C16—C17	120.06 (19)
C5—C6—C7—N2	2.3 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A \cdots O1 ⁱ	0.97	2.43	3.390 (2)	170
C16—H16B \cdots O2 ⁱⁱ	0.97	2.52	3.481 (2)	171

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