

## 6-Bromo-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

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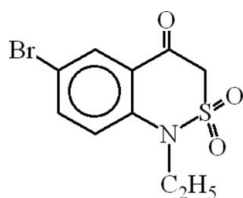
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.095; data-to-parameter ratio = 18.0.

In the title compound,  $\text{C}_{10}\text{H}_{10}\text{BrNO}_3\text{S}$ , the S atom is four-coordinated in a distorted tetrahedral configuration with nearly equal  $\text{S}=\text{O}$  bond distances; the  $\text{S}-\text{C}$  and  $\text{S}-\text{N}$  bond lengths are 1.755 (3) and 1.649 (3) Å, respectively. The heterocyclic thiazine ring adopts a twist conformation. Adjacent molecules are attached to each other through intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming  $R_2^2(8)$  and  $R_2^2(14)$  ring motifs. The molecules are stabilized by intra- and intermolecular hydrogen bonds, forming a three-dimensional polymeric network.

### Related literature

For previous work on benzothiazines, see: Arshad *et al.* (2008); Shafiq, Khan *et al.* (2008); Shafiq, Tahir *et al.* (2008); Tahir *et al.* (2008). For puckering parameters, see: Cremer & Pople (1975). For graph-set motifs, see: Bernstein *et al.* (1995). For synthesis, see: Lombardino (1972).



### Experimental

#### Crystal data

$\text{C}_{10}\text{H}_{10}\text{BrNO}_3\text{S}$

$M_r = 304.16$

Triclinic,  $P\bar{1}$

$a = 7.7164$  (2) Å

$b = 7.9729$  (3) Å

$c = 10.4579$  (3) Å

$\alpha = 86.767$  (2)°

$\beta = 75.773$  (1)°

$\gamma = 66.912$  (2)°

$V = 573.13$  (3) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 3.76$  mm<sup>-1</sup>

$T = 296$  (2) K

$0.28 \times 0.16 \times 0.12$  mm

#### Data collection

Bruker Kappa APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{\min} = 0.486$ ,  $T_{\max} = 0.639$

12369 measured reflections

2846 independent reflections

1840 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.095$

$S = 1.02$

2846 reflections

158 parameters

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.91$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.58$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2}\cdots\text{O1}^{\text{i}}$	0.9300	2.4200	3.324 (4)	165.00
$\text{C3}-\text{H3}\cdots\text{O2}^{\text{ii}}$	0.9300	2.5900	3.418 (4)	148.00
$\text{C8}-\text{H8A}\cdots\text{O3}^{\text{iii}}$	0.89 (4)	2.57 (4)	3.252 (4)	134 (3)
$\text{C9}-\text{H9B}\cdots\text{O3}$	0.93 (3)	2.29 (3)	2.850 (4)	118 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007); 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, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2711).

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## supporting information

*Acta Cryst.* (2009). E65, o393 [doi:10.1107/S1600536809002621]

**6-Bromo-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide**

**Muhammad Shafiq, M. Nawaz Tahir, Islam Ullah Khan, Muhammad Nadeem Arshad and Muhammad Safdar**

**S1. Comment**

Our group is involved in synthesizing various derivatives of benzothiazine molecule (Shafiq, Khan *et al.*, 2008; Shafiq, Tahir *et al.*, 2008; Tahir *et al.*, 2008; Arshad *et al.*, 2008) and their characterization by X-ray studies. We, here, report the title compound (I), (Fig 1), in this context.

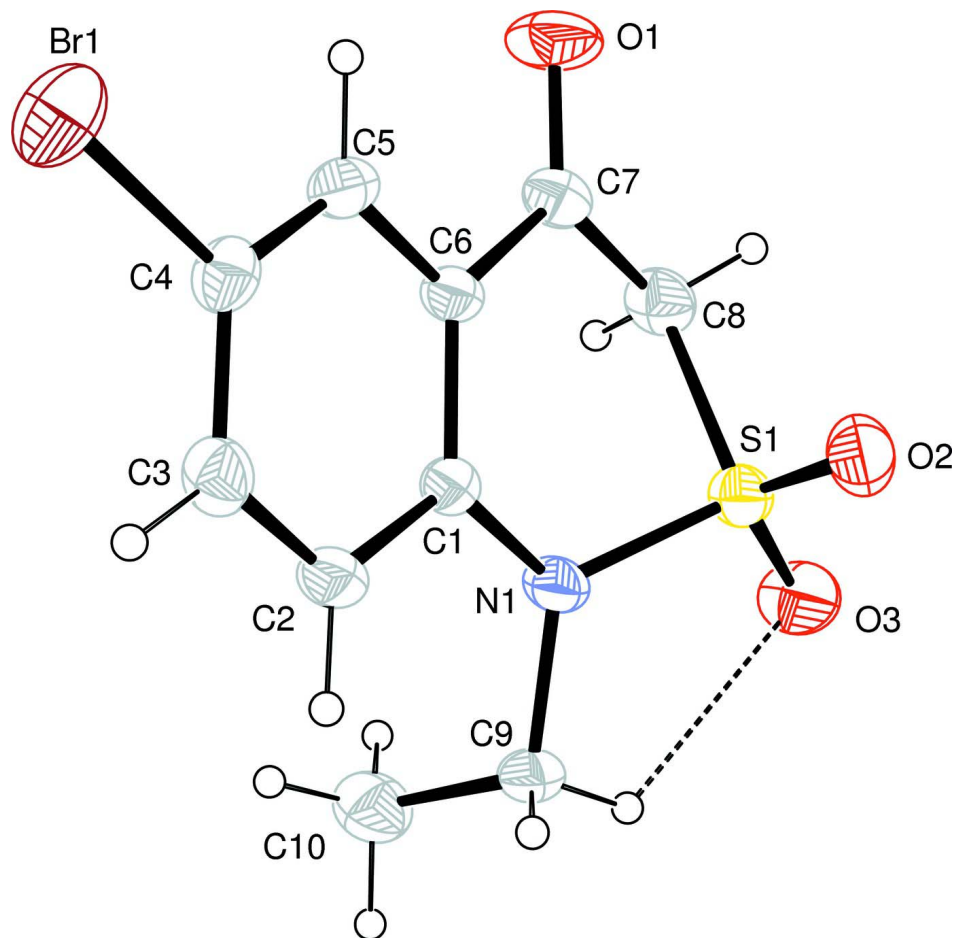
In the title compound, the bromo-substituted benzene ring A (C1–C6), is almost planar with alternate distortions at individual C atoms. The Br atom is at a distance of 0.073 (4) Å from the r.m.s. plane of ring A. The thiazine ring B (S1/N1/C1/C6–C8) is in the twisted form. The maximum puckering (Cremer & Pople, 1975) amplitude,  $Q_T$ , of ring A and ring B is 0.674 (2) Å. There exist an intramolecular H-bond of C—H···O type between the methylene group and the SO<sub>2</sub> moiety. The intermolecular H-bonds [C8—H8A···O3] and [C3—H3···O2] (Table 1), joint the adjacent molecules forming ring motifs, (Bernstein *et al.*, 1995),  $R_2^2(8)$  and  $R_2^2(14)$ , respectively. The three asymmetric units joint in this way, are further linked through [C2—H2···O1] H-bonds with carbonyl moiety (Fig 2).

**S2. Experimental**

The title compound was prepared in a three step scheme following the reported procedure (Lombardino, 1972). Starting material used was methyl-2-amino-5-bromo benzoate. It was reacted with methane sulfonyl chloride taking equimolar quantities, in dichloromethane. The pH was kept alkaline with triethylamine. The product of this step was then *N*-ethylated (ethyl iodide) and cyclized as reported in the above mentioned reference, to get the title compound which was recrystallized in ethanol for X-ray diffraction studies.

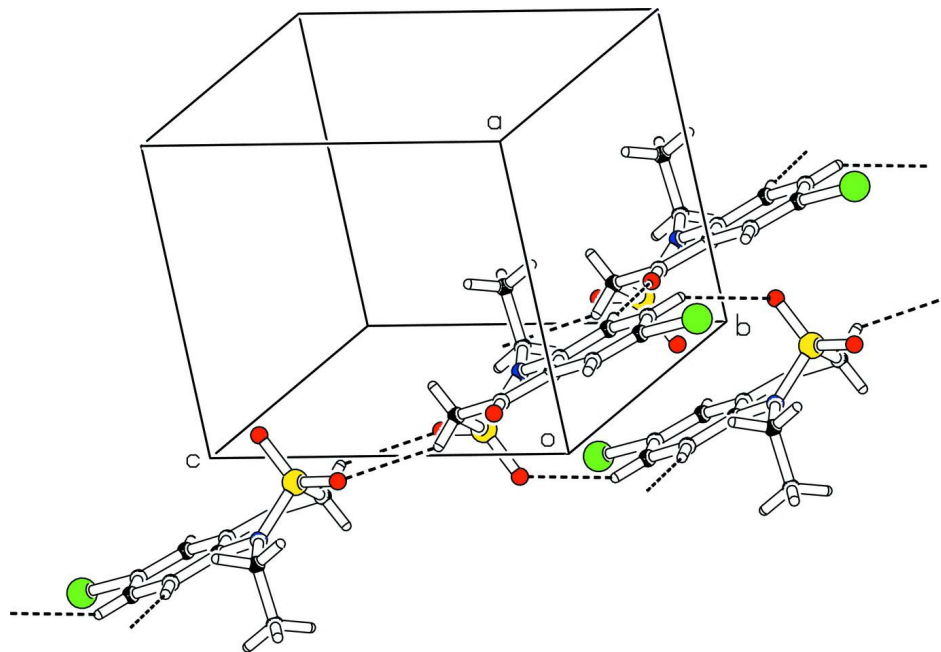
**S3. Refinement**

The H atoms of methylene group were located from a difference Fourier map and refined freely. H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, and constrained to ride on their parent atoms, with  $U_{iso}(H) = xU_{eq}(C)$ , where  $x = 1.5$  for methyl H, and  $x = 1.2$  for all other H atoms.



**Figure 1**

*ORTEP* drawing of the title compound, with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H atoms are shown by small circles of arbitrary radii. The dotted line shows the intramolecular H-bond.

**Figure 2**

The partial packing figure (*PLATON*: Spek, 2003) which shows that intermolecular H-bonds form the ring motifs.

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#### Crystal data

$C_{10}H_{10}BrNO_3S$

$M_r = 304.16$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.7164\ (2)\ \text{\AA}$

$b = 7.9729\ (3)\ \text{\AA}$

$c = 10.4579\ (3)\ \text{\AA}$

$\alpha = 86.767\ (2)^\circ$

$\beta = 75.773\ (1)^\circ$

$\gamma = 66.912\ (2)^\circ$

$V = 573.13\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 304$

$D_x = 1.762\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2847 reflections

$\theta = 2.0\text{--}28.3^\circ$

$\mu = 3.76\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Needle, colourless

$0.28 \times 0.16 \times 0.12\ \text{mm}$

#### Data collection

Bruker Kappa APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution:  $7.40\ \text{pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2005)

$T_{\min} = 0.486$ ,  $T_{\max} = 0.639$

12369 measured reflections

2846 independent reflections

1840 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 28.3^\circ$ ,  $\theta_{\min} = 2.0^\circ$

$h = -10 \rightarrow 9$

$k = -10 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.038$   
 $wR(F^2) = 0.095$   
 $S = 1.02$   
 2846 reflections  
 158 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 atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.3304P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.91 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.36240 (6)	0.15247 (6)	-0.35948 (3)	0.0686 (2)
S1	-0.00069 (12)	0.19519 (10)	0.32296 (7)	0.0435 (3)
O1	0.2170 (4)	-0.2056 (3)	0.0770 (3)	0.0705 (10)
O2	-0.1737 (3)	0.2464 (3)	0.2787 (2)	0.0578 (8)
O3	-0.0156 (4)	0.2267 (3)	0.4583 (2)	0.0668 (10)
N1	0.1437 (4)	0.2891 (3)	0.2351 (2)	0.0450 (9)
C1	0.1999 (4)	0.2535 (4)	0.0977 (3)	0.0358 (9)
C2	0.2376 (5)	0.3826 (4)	0.0126 (3)	0.0444 (10)
C3	0.2876 (5)	0.3511 (4)	-0.1214 (3)	0.0471 (11)
C4	0.3017 (4)	0.1895 (4)	-0.1739 (3)	0.0423 (10)
C5	0.2710 (4)	0.0580 (4)	-0.0934 (3)	0.0416 (10)
C6	0.2210 (4)	0.0869 (4)	0.0432 (3)	0.0361 (9)
C7	0.1935 (4)	-0.0623 (4)	0.1248 (3)	0.0427 (10)
C8	0.1398 (6)	-0.0343 (4)	0.2718 (3)	0.0493 (11)
C9	0.1564 (5)	0.4465 (4)	0.2950 (3)	0.0465 (11)
C10	0.3622 (5)	0.4137 (5)	0.2925 (4)	0.0635 (14)
H2	0.22872	0.49140	0.04727	0.0533*
H3	0.31214	0.43846	-0.17724	0.0564*
H5	0.28342	-0.05116	-0.12983	0.0499*
H8A	0.065 (5)	-0.092 (5)	0.313 (4)	0.0591*
H8B	0.247 (5)	-0.063 (5)	0.306 (3)	0.0591*
H9A	0.092 (5)	0.550 (5)	0.245 (3)	0.0558*
H9B	0.085 (5)	0.457 (4)	0.382 (3)	0.0558*
H10A	0.43344	0.41151	0.20285	0.0948*
H10B	0.36403	0.50981	0.34278	0.0948*

H10C            0.42109                    0.29879                    0.33010                    0.0948\*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0779 (3)	0.0861 (3)	0.0329 (2)	-0.0249 (2)	-0.0092 (2)	0.0002 (2)
S1	0.0540 (5)	0.0443 (4)	0.0344 (4)	-0.0260 (4)	-0.0036 (3)	0.0030 (3)
O1	0.113 (2)	0.0401 (13)	0.0672 (17)	-0.0416 (15)	-0.0168 (15)	-0.0010 (12)
O2	0.0464 (14)	0.0583 (14)	0.0673 (16)	-0.0232 (12)	-0.0074 (12)	0.0063 (12)
O3	0.098 (2)	0.0734 (16)	0.0341 (13)	-0.0463 (15)	-0.0033 (12)	0.0009 (11)
N1	0.0626 (17)	0.0467 (14)	0.0332 (14)	-0.0347 (14)	-0.0012 (12)	-0.0045 (11)
C1	0.0391 (16)	0.0356 (15)	0.0340 (16)	-0.0178 (13)	-0.0056 (12)	-0.0001 (12)
C2	0.0552 (19)	0.0351 (15)	0.0453 (19)	-0.0238 (15)	-0.0057 (15)	0.0010 (13)
C3	0.051 (2)	0.0462 (18)	0.0429 (19)	-0.0212 (16)	-0.0075 (15)	0.0110 (15)
C4	0.0425 (18)	0.0510 (18)	0.0307 (16)	-0.0164 (15)	-0.0074 (13)	0.0015 (14)
C5	0.0439 (18)	0.0377 (16)	0.0418 (18)	-0.0139 (14)	-0.0098 (14)	-0.0056 (14)
C6	0.0419 (17)	0.0324 (15)	0.0369 (16)	-0.0182 (13)	-0.0082 (13)	0.0005 (12)
C7	0.0487 (19)	0.0354 (16)	0.0491 (19)	-0.0198 (14)	-0.0158 (15)	0.0050 (14)
C8	0.061 (2)	0.0436 (18)	0.047 (2)	-0.0254 (18)	-0.0137 (17)	0.0121 (15)
C9	0.056 (2)	0.0423 (17)	0.0440 (19)	-0.0255 (17)	-0.0033 (16)	-0.0115 (15)
C10	0.065 (2)	0.066 (2)	0.071 (3)	-0.033 (2)	-0.023 (2)	-0.004 (2)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Br1—C4	1.893 (3)	C6—C7	1.477 (4)
S1—O2	1.421 (3)	C7—C8	1.496 (4)
S1—O3	1.420 (2)	C9—C10	1.499 (6)
S1—N1	1.649 (3)	C2—H2	0.9300
S1—C8	1.755 (3)	C3—H3	0.9300
O1—C7	1.202 (4)	C5—H5	0.9300
N1—C1	1.406 (4)	C8—H8A	0.89 (4)
N1—C9	1.481 (4)	C8—H8B	0.92 (4)
C1—C2	1.393 (4)	C9—H9A	0.98 (4)
C1—C6	1.409 (4)	C9—H9B	0.93 (3)
C2—C3	1.369 (4)	C10—H10A	0.9600
C3—C4	1.383 (4)	C10—H10B	0.9600
C4—C5	1.364 (4)	C10—H10C	0.9600
C5—C6	1.393 (4)		
Br1 $\cdots$ Br1 <sup>i</sup>	3.5704 (5)	C2 $\cdots$ H9A	2.61 (3)
Br1 $\cdots$ H8B <sup>ii</sup>	3.00 (4)	C2 $\cdots$ H10A	2.8500
O1 $\cdots$ C2 <sup>iii</sup>	3.324 (4)	C9 $\cdots$ H2	2.5500
O2 $\cdots$ C6	3.254 (4)	C10 $\cdots$ H2	2.9400
O2 $\cdots$ C10 <sup>iv</sup>	3.263 (5)	H2 $\cdots$ O1 <sup>ix</sup>	2.4200
O2 $\cdots$ C3 <sup>v</sup>	3.418 (4)	H2 $\cdots$ C9	2.5500
O3 $\cdots$ C8 <sup>vi</sup>	3.252 (4)	H2 $\cdots$ C10	2.9400
O1 $\cdots$ H9A <sup>iii</sup>	2.84 (4)	H2 $\cdots$ H9A	2.0600
O1 $\cdots$ H2 <sup>iii</sup>	2.4200	H2 $\cdots$ H10A	2.4300

O1...H5	2.4700	H3...O2 <sup>v</sup>	2.5900
O2...H10C <sup>iv</sup>	2.9000	H5...O1	2.4700
O2...H5 <sup>vii</sup>	2.7400	H5...O2 <sup>vii</sup>	2.7400
O2...H3 <sup>v</sup>	2.5900	H8A...O3 <sup>vi</sup>	2.57 (4)
O3...H9B	2.29 (3)	H8B...Br1 <sup>ii</sup>	3.00 (4)
O3...H8A <sup>vi</sup>	2.57 (4)	H9A...O1 <sup>ix</sup>	2.84 (4)
O3...H9B <sup>viii</sup>	2.90 (3)	H9A...C2	2.61 (3)
C2...O1 <sup>ix</sup>	3.324 (4)	H9A...H2	2.0600
C2...C10	3.348 (5)	H9B...O3	2.29 (3)
C2...C2 <sup>v</sup>	3.472 (5)	H9B...O3 <sup>viii</sup>	2.90 (3)
C3...O2 <sup>v</sup>	3.418 (4)	H9B...H9B <sup>viii</sup>	2.49 (4)
C6...O2	3.254 (4)	H10A...C1	2.9900
C8...O3 <sup>vi</sup>	3.252 (4)	H10A...C2	2.8500
C10...C2	3.348 (5)	H10A...H2	2.4300
C10...O2 <sup>x</sup>	3.263 (5)	H10C...O2 <sup>x</sup>	2.9000
C1...H10A	2.9900		
O2—S1—O3	118.87 (16)	S1—C8—C7	112.1 (2)
O2—S1—N1	110.91 (14)	N1—C9—C10	111.6 (3)
O2—S1—C8	106.97 (18)	C1—C2—H2	120.00
O3—S1—N1	107.50 (16)	C3—C2—H2	120.00
O3—S1—C8	111.51 (15)	C2—C3—H3	120.00
N1—S1—C8	99.36 (16)	C4—C3—H3	120.00
S1—N1—C1	117.1 (2)	C4—C5—H5	120.00
S1—N1—C9	118.39 (19)	C6—C5—H5	120.00
C1—N1—C9	121.6 (2)	S1—C8—H8A	104 (2)
N1—C1—C2	120.3 (3)	S1—C8—H8B	104 (2)
N1—C1—C6	121.0 (3)	C7—C8—H8A	113 (3)
C2—C1—C6	118.7 (3)	C7—C8—H8B	112 (2)
C1—C2—C3	120.7 (3)	H8A—C8—H8B	111 (3)
C2—C3—C4	120.1 (3)	N1—C9—H9A	104 (2)
Br1—C4—C3	119.3 (2)	N1—C9—H9B	105 (2)
Br1—C4—C5	120.0 (2)	C10—C9—H9A	115 (2)
C3—C4—C5	120.7 (3)	C10—C9—H9B	110 (3)
C4—C5—C6	120.1 (3)	H9A—C9—H9B	111 (3)
C1—C6—C5	119.6 (3)	C9—C10—H10A	109.00
C1—C6—C7	122.9 (3)	C9—C10—H10B	110.00
C5—C6—C7	117.4 (3)	C9—C10—H10C	109.00
O1—C7—C6	122.2 (3)	H10A—C10—H10B	109.00
O1—C7—C8	119.4 (3)	H10A—C10—H10C	109.00
C6—C7—C8	118.4 (3)	H10B—C10—H10C	109.00
O2—S1—N1—C1	-56.8 (3)	N1—C1—C6—C5	178.0 (3)
O2—S1—N1—C9	104.3 (2)	N1—C1—C6—C7	-2.4 (5)
O3—S1—N1—C1	171.7 (2)	C2—C1—C6—C5	-2.6 (5)
O3—S1—N1—C9	-27.2 (3)	C2—C1—C6—C7	177.1 (3)
C8—S1—N1—C1	55.5 (3)	C1—C2—C3—C4	-0.2 (6)
C8—S1—N1—C9	-143.4 (3)	C2—C3—C4—Br1	177.9 (3)

O2—S1—C8—C7	61.0 (3)	C2—C3—C4—C5	-1.7 (6)
O3—S1—C8—C7	-167.5 (3)	Br1—C4—C5—C6	-178.2 (3)
N1—S1—C8—C7	-54.3 (3)	C3—C4—C5—C6	1.3 (5)
S1—N1—C1—C2	149.4 (3)	C4—C5—C6—C1	0.8 (5)
S1—N1—C1—C6	-31.2 (4)	C4—C5—C6—C7	-178.8 (3)
C9—N1—C1—C2	-11.1 (5)	C1—C6—C7—O1	-178.0 (3)
C9—N1—C1—C6	168.3 (3)	C1—C6—C7—C8	0.4 (5)
S1—N1—C9—C10	125.2 (3)	C5—C6—C7—O1	1.7 (5)
C1—N1—C9—C10	-74.6 (4)	C5—C6—C7—C8	180.0 (3)
N1—C1—C2—C3	-178.3 (3)	O1—C7—C8—S1	-150.2 (3)
C6—C1—C2—C3	2.2 (5)	C6—C7—C8—S1	31.4 (5)

Symmetry codes: (i)  $-x+1, -y, -z-1$ ; (ii)  $-x+1, -y, -z$ ; (iii)  $x, y-1, z$ ; (iv)  $x-1, y, z$ ; (v)  $-x, -y+1, -z$ ; (vi)  $-x, -y, -z+1$ ; (vii)  $-x, -y, -z$ ; (viii)  $-x, -y+1, -z+1$ ; (ix)  $x, y+1, z$ ; (x)  $x+1, y, z$ .

*Hydrogen-bond geometry (Å, °)*

<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>
C2—H2...O1 <sup>ix</sup>	0.9300	2.4200	3.324 (4)	165.00
C3—H3...O2 <sup>v</sup>	0.9300	2.5900	3.418 (4)	148.00
C8—H8 <i>A</i> ...O3 <sup>vi</sup>	0.89 (4)	2.57 (4)	3.252 (4)	134 (3)
C9—H9 <i>B</i> ...O3	0.93 (3)	2.29 (3)	2.850 (4)	118 (2)

Symmetry codes: (v)  $-x, -y+1, -z$ ; (vi)  $-x, -y, -z+1$ ; (ix)  $x, y+1, z$ .