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3-Butyl-2-phenyl-1,3-thiazolidine-1,4-dione

Qiang Wang,[a]* Zhouqin Xu[a] and Yanchun Sun[b]

[a]Department of Physics–Chemistry, Henan Polytechnic University, Jiao Zuo 454000, People's Republic of China, and [b]Department of Medicine, Hebi College of Vocation and Technology, He Bi 458030, People's Republic of China
Correspondence e-mail: wangqiang@hpu.edu.cn

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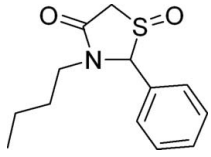
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.159; data-to-parameter ratio = 20.1.

In the title compound, $C_{13}H_{17}NO_2S$, the thiazolidine-1,4-dione ring adopts an envelope conformation with the S atom lying 0.631 (4) Å out of the plane formed by the other four ring atoms; the phenyl ring is almost perpendicular [88.74 (8)°] with respect to the ring C—C—N—C atoms and the butyl chain is in a fully extended conformation. In the crystal, a supramolecular two-dimensional arrangement arises from weak intermolecular C—H···O interactions.

Related literature

For related structures, see: Wang *et al.* (2009); Xu *et al.* (2009). For synthetic procedures, see: Johnson *et al.* (1983); Srivastava *et al.* (2002).



Experimental

Crystal data

$C_{13}H_{17}NO_2S$
M_r = 251.34
Monoclinic, $P2_1/c$
a = 13.8335 (5) Å
b = 8.7461 (3) Å
c = 12.3853 (4) Å
β = 114.773 (2)°
V = 1360.59 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 297 K
0.28 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.939, T_{max} = 0.956
15990 measured reflections
3118 independent reflections
2169 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.159
S = 1.14
3118 reflections
155 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O1^{i}	0.97	2.43	3.246 (3)	142
C3—H3···O2^{ii}	0.98	2.34	3.311 (3)	172
C11—H11B···O2^{ii}	0.97	2.59	3.548 (4)	169

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2278).

References

Bruker (2001). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, M. R., Dong, M., Fazio, M. J., Ward, D. L. & Sousa, L. R. (1983). *J. Org. Chem.* **48**, 494–499.
Sheldrick, G. M. (1997). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Srivastava, T., Haq, W. & Katti, S. B. (2002). *Tetrahedron*, **58**, 7619–7624.
Wang, Q., Yang, L., Xu, Z. & Sun, Y. (2009). *Acta Cryst.* E**65**, o1978.
Xu, Z., Sun, Y., Yang, L. & Wang, Q. (2009). *Acta Cryst.* E**65**, o1799.

supporting information

Acta Cryst. (2010). E**66**, o1422 [https://doi.org/10.1107/S1600536810018003]

3-Butyl-2-phenyl-1,3-thiazolidine-1,4-dione

Qiang Wang, Zhouqin Xu and Yanchun Sun

S1. Comment

As a part of our programme studying the new applications of cyclic sulfoxide derivatives in medicne (Wang, *et al.*, 2009; Xu, *et al.*, 2009), we report herein the crystal structure of the title compounds.

The molecular structure of the title compound is shown in Fig. 1. The thiazolidin-4-one ring adopts an envelope conformation with S lying 0.631 (4) Å out of the plane formed by the rest of the ring atoms; the phenyl ring is oriented at right angles (88.74 (8)°) with respect to the ring (C2/C3/N1/C1) atoms. The butyl chain is in a fully extended conformation. The crystal packing (Fig. 2) consists of a two-dimensional network in the *a*-*c*-plane generated by intermolecular interactions of the weak C—H···O hydrogen bonds.

S2. Experimental

All reagents were of analytical grade. The title compound was prepared according to literature methods (Srivastava *et al.*, 2002; Johnson *et al.*, 1983). It was characterized by recording its infrared spectra and elemental analyses. Single crystals of the title compound were obtained by slow evaporation of its chloroform solution at room temperature.

S3. Refinement

All H atoms bonded to C atoms were calculated in idealized position with C—H = 0.93-0.98 Å and refined in riding mode on their parent atoms with U_{iso}(H) values of 1.2U_{eq}(C).

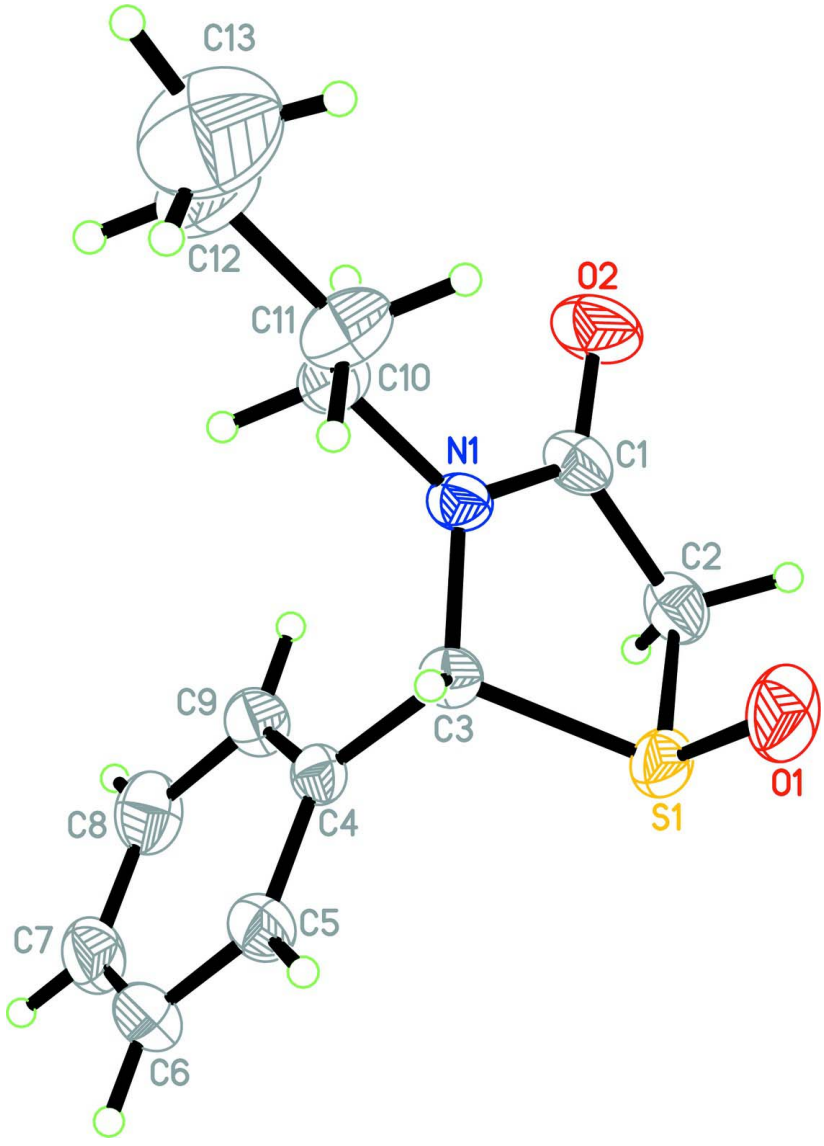

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

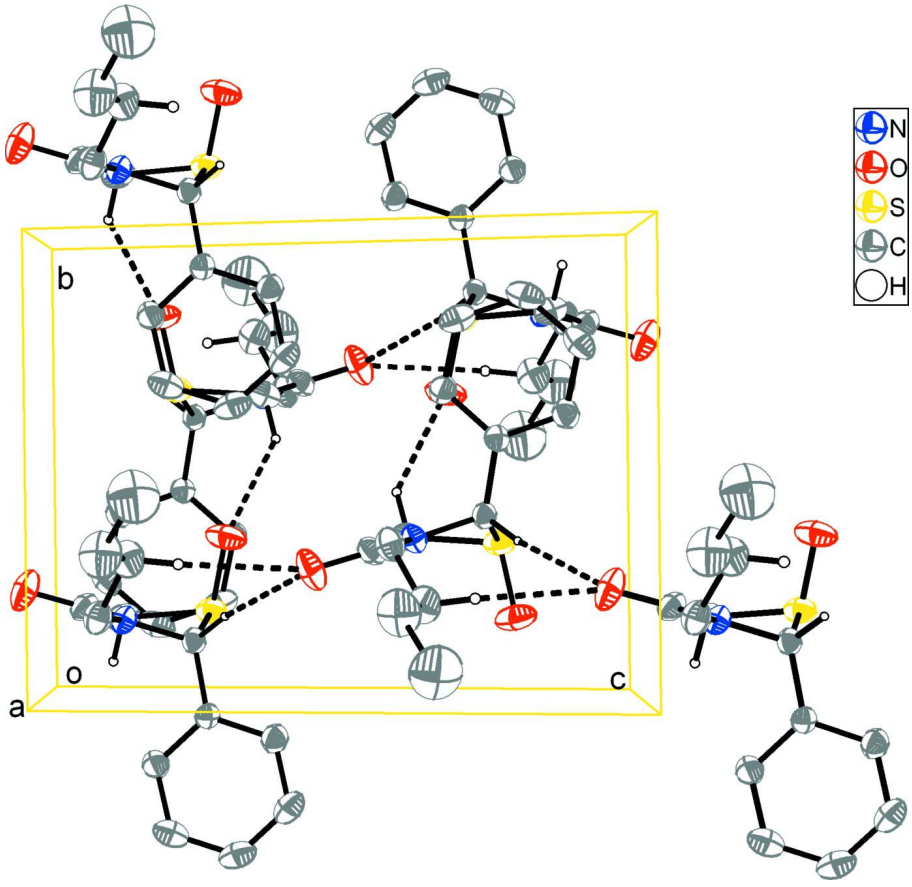

Figure 2

A view of the unit cell packing of the title compound down the *a*-axis showing hydrogen bonds as dashed lines.

3-Butyl-2-phenyl-1,3-thiazolidine-1,4-dione

Crystal data

$C_{13}H_{17}NO_2S$
$M_r = 251.34$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.8335$ (5) Å
$b = 8.7461$ (3) Å
$c = 12.3853$ (4) Å
$\beta = 114.773$ (2)°
$V = 1360.59$ (8) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.227$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5947 reflections
$\theta = 2.8$–25.9°
$\mu = 0.23$ mm^{-1}
$T = 297$ K
Block, yellow
0.28 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{min} = 0.939$, $T_{max} = 0.956$
15990 measured reflections
3118 independent reflections
2169 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = -17 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.159$
$S = 1.14$
3118 reflections
155 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2 + 0.1042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ 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 $F^2 > \sigma(F^2)$ 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}
N1	0.25227 (13)	0.66161 (18)	0.36775 (14)	0.0437 (4)
O1	0.04410 (14)	0.84045 (17)	0.19284 (19)	0.0788 (6)
O2	0.24851 (16)	0.7278 (2)	0.54296 (16)	0.0820 (6)
S1	0.04960 (4)	0.67497 (6)	0.22013 (5)	0.0522 (2)
C1	0.20313 (18)	0.6887 (2)	0.4393 (2)	0.0514 (5)
C2	0.08545 (18)	0.6614 (2)	0.3755 (2)	0.0553 (6)
H2A	0.0469	0.7371	0.3993	0.066*
H2B	0.0678	0.5608	0.3949	0.066*
C3	0.18626 (14)	0.6127 (2)	0.24789 (16)	0.0410 (5)
H3	0.2085	0.6679	0.1933	0.049*
C4	0.18891 (14)	0.4445 (2)	0.22558 (16)	0.0393 (4)
C5	0.15706 (17)	0.3929 (2)	0.10953 (19)	0.0525 (5)
H5	0.1360	0.4631	0.0474	0.063*
C6	0.1564 (2)	0.2395 (3)	0.0856 (2)	0.0650 (7)
H6	0.1346	0.2067	0.0075	0.078*
C7	0.1875 (2)	0.1350 (3)	0.1756 (3)	0.0692 (7)
H7	0.1875	0.0313	0.1589	0.083*
C8	0.2186 (2)	0.1831 (3)	0.2906 (3)	0.0677 (7)
H8	0.2387	0.1118	0.3518	0.081*
C9	0.22036 (17)	0.3375 (2)	0.3161 (2)	0.0531 (6)
H9	0.2428	0.3694	0.3945	0.064*
C10	0.36729 (17)	0.6710 (3)	0.4092 (2)	0.0577 (6)
H10A	0.3932	0.5761	0.3906	0.069*
H10B	0.3996	0.6830	0.4949	0.069*
C11	0.4012 (2)	0.8007 (3)	0.3546 (3)	0.0734 (7)

H11A	0.3744	0.8954	0.3726	0.088*
H11B	0.3689	0.7882	0.2689	0.088*
C12	0.5200 (2)	0.8135 (4)	0.3968 (3)	0.1025 (11)
H12A	0.5521	0.8311	0.4820	0.123*
H12B	0.5473	0.7173	0.3821	0.123*
C13	0.5527 (3)	0.9381 (6)	0.3380 (4)	0.1532 (17)
H13A	0.5328	0.9122	0.2561	0.184*
H13B	0.6284	0.9516	0.3773	0.184*
H13C	0.5179	1.0314	0.3425	0.184*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0431 (9)	0.0507 (10)	0.0389 (9)	−0.0063 (7)	0.0189 (7)	−0.0076 (7)
O1	0.0751 (12)	0.0415 (10)	0.1114 (15)	0.0132 (7)	0.0307 (11)	0.0173 (9)
O2	0.0877 (14)	0.1101 (16)	0.0556 (11)	−0.0193 (11)	0.0372 (10)	−0.0332 (10)
S1	0.0453 (3)	0.0400 (3)	0.0641 (4)	0.0035 (2)	0.0156 (3)	0.0018 (2)
C1	0.0614 (14)	0.0500 (12)	0.0506 (14)	−0.0080 (10)	0.0312 (11)	−0.0118 (10)
C2	0.0566 (13)	0.0484 (12)	0.0733 (16)	−0.0076 (9)	0.0395 (12)	−0.0104 (10)
C3	0.0437 (10)	0.0447 (10)	0.0367 (11)	−0.0019 (8)	0.0190 (9)	0.0008 (8)
C4	0.0381 (10)	0.0426 (10)	0.0403 (11)	0.0019 (8)	0.0195 (8)	−0.0010 (8)
C5	0.0572 (13)	0.0567 (13)	0.0464 (13)	0.0022 (10)	0.0243 (10)	−0.0042 (10)
C6	0.0661 (16)	0.0669 (16)	0.0636 (16)	−0.0004 (12)	0.0288 (13)	−0.0227 (13)
C7	0.0654 (15)	0.0489 (13)	0.094 (2)	0.0026 (11)	0.0339 (15)	−0.0165 (14)
C8	0.0723 (17)	0.0492 (14)	0.083 (2)	0.0130 (11)	0.0336 (14)	0.0151 (12)
C9	0.0617 (14)	0.0517 (12)	0.0472 (13)	0.0068 (10)	0.0241 (11)	0.0037 (9)
C10	0.0464 (12)	0.0706 (15)	0.0527 (14)	−0.0020 (10)	0.0174 (10)	−0.0063 (11)
C11	0.0514 (15)	0.0891 (18)	0.0734 (18)	−0.0103 (13)	0.0200 (13)	0.0048 (14)
C12	0.0567 (17)	0.137 (3)	0.113 (3)	−0.0209 (17)	0.0347 (18)	−0.005 (2)
C13	0.127 (2)	0.179 (3)	0.168 (3)	−0.041 (2)	0.076 (2)	0.009 (2)

Geometric parameters (Å, º)

N1—C1	1.345 (2)	C7—C8	1.370 (4)
N1—C3	1.444 (2)	C7—H7	0.9300
N1—C10	1.455 (3)	C8—C9	1.385 (3)
O1—S1	1.4809 (16)	C8—H8	0.9300
O2—C1	1.218 (3)	C9—H9	0.9300
S1—C2	1.779 (2)	C10—C11	1.493 (3)
S1—C3	1.8559 (18)	C10—H10A	0.9700
C1—C2	1.501 (3)	C10—H10B	0.9700
C2—H2A	0.9700	C11—C12	1.507 (4)
C2—H2B	0.9700	C11—H11A	0.9700
C3—C4	1.500 (3)	C11—H11B	0.9700
C3—H3	0.9800	C12—C13	1.482 (5)
C4—C9	1.383 (3)	C12—H12A	0.9700
C4—C5	1.390 (3)	C12—H12B	0.9700
C5—C6	1.374 (3)	C13—H13A	0.9600

C5—H5	0.9300	C13—H13B	0.9600
C6—C7	1.364 (4)	C13—H13C	0.9600
C6—H6	0.9300		

C1—N1—C3	116.95 (17)	C8—C7—H7	120.1
C1—N1—C10	122.52 (18)	C7—C8—C9	120.3 (2)
C3—N1—C10	120.42 (15)	C7—C8—H8	119.8
O1—S1—C2	106.05 (11)	C9—C8—H8	119.8
O1—S1—C3	106.27 (10)	C8—C9—C4	120.3 (2)
C2—S1—C3	88.82 (9)	C8—C9—H9	119.8
O2—C1—N1	124.4 (2)	C4—C9—H9	119.8
O2—C1—C2	124.46 (19)	N1—C10—C11	112.81 (18)
N1—C1—C2	111.17 (19)	N1—C10—H10A	109.0
C1—C2—S1	107.95 (14)	C11—C10—H10A	109.0
C1—C2—H2A	110.1	N1—C10—H10B	109.0
S1—C2—H2A	110.1	C11—C10—H10B	109.0
C1—C2—H2B	110.1	H10A—C10—H10B	107.8
S1—C2—H2B	110.1	C10—C11—C12	113.8 (2)
H2A—C2—H2B	108.4	C10—C11—H11A	108.8
N1—C3—C4	115.24 (16)	C12—C11—H11A	108.8
N1—C3—S1	105.05 (12)	C10—C11—H11B	108.8
C4—C3—S1	110.82 (12)	C12—C11—H11B	108.8
N1—C3—H3	108.5	H11A—C11—H11B	107.7
C4—C3—H3	108.5	C13—C12—C11	113.4 (3)
S1—C3—H3	108.5	C13—C12—H12A	108.9
C9—C4—C5	118.34 (19)	C11—C12—H12A	108.9
C9—C4—C3	122.52 (18)	C13—C12—H12B	108.9
C5—C4—C3	119.13 (17)	C11—C12—H12B	108.9
C6—C5—C4	120.7 (2)	H12A—C12—H12B	107.7
C6—C5—H5	119.6	C12—C13—H13A	109.5
C4—C5—H5	119.6	C12—C13—H13B	109.5
C7—C6—C5	120.5 (2)	H13A—C13—H13B	109.5
C7—C6—H6	119.8	C12—C13—H13C	109.5
C5—C6—H6	119.8	H13A—C13—H13C	109.5
C6—C7—C8	119.8 (2)	H13B—C13—H13C	109.5
C6—C7—H7	120.1		

C3—N1—C1—O2	178.6 (2)	N1—C3—C4—C9	21.3 (3)
C10—N1—C1—O2	2.4 (3)	S1—C3—C4—C9	−97.9 (2)
C3—N1—C1—C2	−0.3 (2)	N1—C3—C4—C5	−159.80 (16)
C10—N1—C1—C2	−176.47 (18)	S1—C3—C4—C5	81.10 (18)
O2—C1—C2—S1	159.4 (2)	C9—C4—C5—C6	0.3 (3)
N1—C1—C2—S1	−21.8 (2)	C3—C4—C5—C6	−178.67 (18)
O1—S1—C2—C1	−78.65 (16)	C4—C5—C6—C7	−0.2 (3)
C3—S1—C2—C1	27.94 (15)	C5—C6—C7—C8	0.6 (4)
C1—N1—C3—C4	−101.4 (2)	C6—C7—C8—C9	−1.0 (4)
C10—N1—C3—C4	74.9 (2)	C7—C8—C9—C4	1.1 (3)
C1—N1—C3—S1	20.9 (2)	C5—C4—C9—C8	−0.7 (3)

C10—N1—C3—S1	−162.82 (15)	C3—C4—C9—C8	178.21 (18)
O1—S1—C3—N1	78.93 (14)	C1—N1—C10—C11	−112.5 (2)
C2—S1—C3—N1	−27.45 (13)	C3—N1—C10—C11	71.4 (2)
O1—S1—C3—C4	−155.99 (14)	N1—C10—C11—C12	179.6 (2)
C2—S1—C3—C4	97.63 (14)	C10—C11—C12—C13	177.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O1^{i}	0.97	2.43	3.246 (3)	142
C3—H3···O2^{ii}	0.98	2.34	3.311 (3)	172
C9—H9···N1	0.93	2.59	2.899 (2)	100
C10—H10*B*···O2	0.97	2.43	2.824 (3)	104
C11—H11*B*···O2^{ii}	0.97	2.59	3.548 (4)	169

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2.