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(*Z*)-3-Butyl-5-(4-nitrobenzylidene)thiazolidine-2,4-dione

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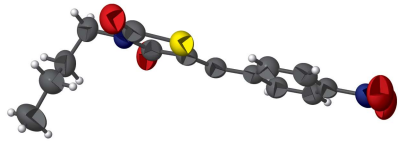
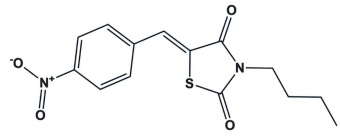
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{14}N_2O_4S$, the benzene and thiazolidine rings are almost coplanar with a dihedral angle of 2.98 (14)°. The butyl chain is directed almost perpendicular to the plane of the rest of the molecule. In the crystal, a combination of C—H···O hydrogen bonds and offset π–π interactions leads to the formation of a three-dimensional structure.

3D view



Chemical scheme



Structure description

Thiazolidines are an important class of heteroaromatic compounds and have widespread applications from pharmaceuticals (Barreca *et al.*, 2002) to materials (Botti *et al.*, 1996). Substituted thiazolidine derivatives represent important key intermediates for the synthesis of pharmacologically active drugs. The group has a wide range of biological activities such as antifungal, antiproliferative, anti-inflammatory, antimalarial, herbicidal, antiviral (Samadhiya *et al.*, 2012), anti-convulsant (Pandey *et al.*, 2011), anticancer and anti-oxidant, and also has interesting antimicrobial activity (influenza). In addition, antidiabetic properties (Majed & Abid, 2015) have been reported. There are numerous biologically active molecules with five-membered rings containing two hetero atoms. Among them, thiazolidines are the most extensively investigated class of compounds (Fun *et al.*, 2011). Thiazolidine derivatives exhibit anti-HIV, antituberculotic (Fun *et al.*, 2011), herbicidal, antineoplastic, hypolipidemic and anti-inflammatory activities (Vennila *et al.*, 2011). Thiazolidines have many interesting activity profiles, namely as COX-1 inhibitors, inhibitors of the bacterial enzyme MurB, which is a precursor, acting during the biosynthesis of peptidoglycan, non-nucleoside inhibitors of HIV–RT and anti-hista-

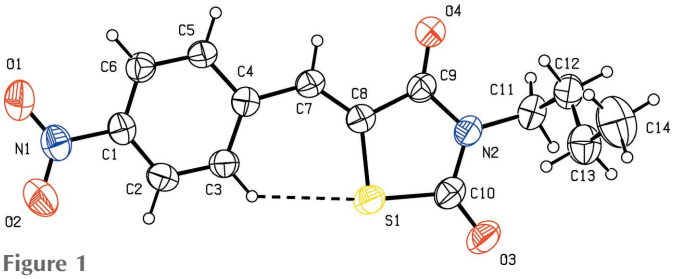


Figure 1
A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular C—H···S interaction (see Table 1) is shown as a dashed line.

minic agents (Čačić *et al.*, 2010). The presence of a thiazolidine ring in penicillin and related derivatives was the first recognition of its occurrence in nature (Čačić *et al.*, 2010).

The molecular structure of the title compound is shown in Fig. 1. The benzene and thiazolidinedione rings are inclined to each other by 2.98 (14)° and there is an intramolecular C—H···S interaction present forming an *S*(6) ring motif (Fig. 1 and Table 1). The configuration about the C7=C8 bond is *Z*. The butyl chain is in a fully extended conformation and oriented normal to the thiazolidinedione ring plane (Fig. 1).

In the crystal, molecules are linked by C—H···O hydrogen bonds, forming rectangular panels lying parallel to the *bc* plane (Fig. 2 and Table 1). The bulky aliphatic substituents are oriented out of the plane of the molecule to occupy the space between the panels (Figs. 2 and 3). The panels are linked by offset π–π interactions involving inversion-related benzene rings, so forming a three-dimensional structure [$Cg2\cdots Cg2^{iv}$ = 3.882 (2) Å, $Cg2$ is the centroid of the C1–C6 ring, α = 0.00 (14), β = 25.6°, interplanar distance = 3.503 (1) Å, offset = 1.675 Å, symmetry code (iv): $-x+1, -y+1, -z+1$].

A search of the Cambridge Structural Database (CSD, version 5.39, update May 2018; Groom *et al.*, 2016) for 5-(benzylidene)-thiazolidine-2,4-diones gave 12 hits. The compounds closest to the title compound are ethyl [(5*Z*)-5-(4-methylbenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl] acetate (CSD refcode APAJEI; Khalid *et al.*, 2016) and ethyl [(5*Z*)-5-(4-methoxybenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl] acetate (IQUHIN; Tachallait *et al.*, 2016). As in the title compound, there is an intramolecular C—H···S interaction present in both compounds, and the benzene and thiazolidine rings are inclined to each other by 5.33 (8) and 1.49 (6)°, respectively, compared to 2.98 (14)° in the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···S1	0.93	2.55	3.256 (3)	133
C2—H2···O4^{i}	0.93	2.45	3.139 (4)	131
C5—H5···O2^{ii}	0.93	2.60	3.468 (4)	156
C11—H11*B*···O3^{iii}	0.97	2.60	3.281 (3)	128

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

Synthesis and crystallization

An aqueous solution (15 ml) of chloroacetic acid (0.075 *M*) was placed in a 100 ml round-bottom flask and thiourea (0.075 *M*) was added with continuous stirring for 20 min. The reaction mixture was refluxed for 40 h at 373–383 K. On cooling, the contents of the flask solidified into a white needle-like product. This product was filtered and washed with a sufficient amount of water to remove untreated substrates. It was dried and recrystallized with methanol to get pure thiazolidine-2,4-dione. A stirred solution of thiazolidine-2,4-dione (9 mmol) in 20 ml glacial acetic acid was buffered with sodium acetate (18 mmol) followed by the addition of 4-nitrobenzaldehyde (9 mmol), then refluxed with stirring for 6 h for Knoevenagel's condensation. The final reaction mixture was poured into ice-cold water, resulting in the precipitation of 5-(4-nitrobenzylidene)thiazolidine-2,4-dione. The precipitate was filtered through a Buchner funnel and thoroughly washed with cold water. Finally, recrystallization was achieved with methanol, and the recrystallized product was dried in a vacuum desiccator over fused calcium chloride. In the last step, the product (4.5 mmol) was dissolved in 30 ml of anhydrous DMF and solid sodium hydride (20 mmol) was slowly added. The reaction mixture was stirred at ambient temperature until hydrogen gas bubbles had stopped. The transparent solution with suspended sodium hydride particles was filtered. The

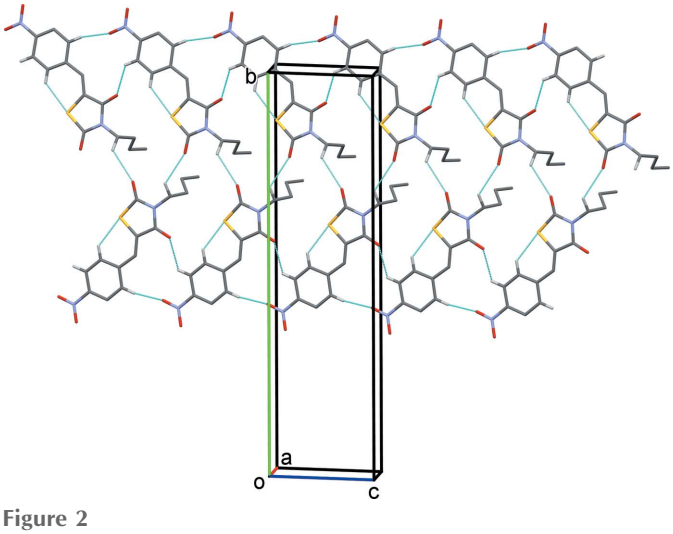


Figure 2
A partial view along the *a* axis of the crystal packing of the title compound. Dashed lines indicate hydrogen bonds (Table 1) and H atoms not involved in these interactions have been omitted.

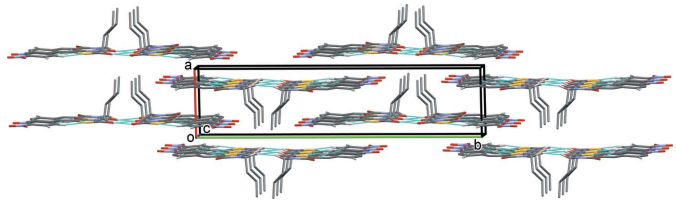


Figure 3
A view along the *c* axis of the crystal packing of the title compound. Dashed lines indicate hydrogen bonds (Table 1) and H atoms not involved in these interactions have been omitted.

filtrate was added dropwise to a solution of 1-chlorobutane (11.25 mmol in 20 ml of anhydrous DMF). The resulting reaction mixture was stirred at ambient temperature under a nitrogen atmosphere for 1 h. The solvent was removed, and the residue washed with hexane several times to remove any excess of 1-chlorobutane. Finally, the product was dried overnight under vacuum in a vacuum desiccator over fused calcium chloride. The compound was then dissolved in methanol and fine needle-like crystals of the title compound were obtained after two days on slow evaporation of the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}N_2O_4S$
M_r	306.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	7.2595 (8), 27.492 (3), 7.9630 (9)
β (°)	113.072 (8)
V (Å^3)	1462.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.74 × 0.54 × 0.28
Data collection	
Diffractometer	Stoe *IPDS* 2
Absorption correction	Integration (*X-RED32* and *X-SHAPE*; Stoe & Cie, 2017)
T_{min}, T_{max}	0.833, 0.936
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8120, 2855, 1430
R_{int}	0.078
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.141, 0.83
No. of reflections	2855
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.22

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2017), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2019). **4**, x190094 [https://doi.org/10.1107/S2414314619000944]

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Crystal data

$C_{14}H_{14}N_2O_4S$
M_r = 306.33
Monoclinic, $P2_1/c$
a = 7.2595 (8) Å
b = 27.492 (3) Å
c = 7.9630 (9) Å
β = 113.072 (8)°
V = 1462.1 (3) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9040 reflections
θ = 1.5–27.5°
μ = 0.24 mm^{-1}
T = 296 K
Prism, yellow
0.74 × 0.54 × 0.28 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32 & X-SHAPE; Stoe & Cie, 2017)
T_{min} = 0.833, T_{max} = 0.936
8120 measured reflections
2855 independent reflections
1430 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 26.0°, θ_{min} = 1.5°
h = −8→8
k = −33→33
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.141
S = 0.83
2855 reflections
191 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
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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. H atoms were positioned geometrically and refined as riding: C—H = 0.95–0.98 Å with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.24335 (11)	0.62282 (3)	0.56254 (11)	0.0773 (3)
O4	0.2873 (3)	0.57655 (7)	1.0303 (3)	0.0904 (6)
N2	0.2667 (3)	0.64894 (8)	0.8866 (3)	0.0700 (6)
O3	0.2360 (3)	0.71142 (7)	0.6862 (3)	0.1027 (7)
N1	0.2171 (4)	0.40379 (12)	0.1189 (4)	0.0844 (7)
O1	0.2111 (4)	0.36052 (9)	0.1416 (4)	0.1175 (9)
C4	0.2562 (3)	0.49850 (9)	0.5495 (3)	0.0611 (6)
C9	0.2755 (4)	0.59888 (10)	0.8958 (4)	0.0673 (7)
C5	0.2708 (4)	0.44824 (9)	0.5746 (4)	0.0665 (7)
H5	0.290385	0.435385	0.688347	0.080*
C8	0.2653 (3)	0.57709 (9)	0.7210 (3)	0.0621 (6)
C1	0.2298 (4)	0.43668 (10)	0.2678 (4)	0.0665 (7)
C2	0.2147 (4)	0.48596 (11)	0.2365 (4)	0.0723 (7)
H2	0.196410	0.498308	0.122312	0.087*
O2	0.2101 (4)	0.42141 (11)	−0.0246 (4)	0.1234 (9)
C7	0.2705 (3)	0.52875 (9)	0.7049 (4)	0.0643 (7)
H7	0.285820	0.511529	0.810095	0.077*
C3	0.2272 (4)	0.51661 (10)	0.3763 (4)	0.0687 (7)
H3	0.216151	0.549995	0.355939	0.082*
C6	0.2567 (4)	0.41738 (10)	0.4346 (4)	0.0700 (7)
H6	0.265227	0.383898	0.452533	0.084*
C10	0.2485 (4)	0.66871 (10)	0.7210 (4)	0.0763 (8)
C12	0.4807 (5)	0.68443 (11)	1.1853 (4)	0.0922 (10)
H12A	0.472121	0.698510	1.293761	0.111*
H12B	0.541145	0.652509	1.217739	0.111*
C11	0.2710 (4)	0.67873 (10)	1.0404 (4)	0.0838 (9)
H11A	0.186205	0.663844	1.094628	0.101*
H11B	0.216699	0.710631	0.995844	0.101*
C13	0.6140 (5)	0.71590 (13)	1.1259 (5)	0.1011 (10)
H13A	0.559680	0.748613	1.102842	0.121*
H13B	0.615268	0.703279	1.012595	0.121*
C14	0.8259 (6)	0.71780 (18)	1.2675 (6)	0.1483 (17)
H14A	0.904272	0.739189	1.226608	0.222*
H14B	0.882969	0.685760	1.285421	0.222*
H14C	0.825022	0.729644	1.380650	0.222*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0841 (5)	0.0659 (4)	0.0764 (5)	−0.0032 (4)	0.0254 (4)	0.0078 (4)
O4	0.1288 (17)	0.0698 (12)	0.0784 (14)	−0.0099 (11)	0.0470 (13)	−0.0031 (11)
N2	0.0716 (14)	0.0561 (13)	0.0759 (16)	−0.0010 (10)	0.0219 (12)	−0.0029 (11)

O3	0.1218 (19)	0.0604 (12)	0.1050 (17)	0.0011 (12)	0.0217 (14)	0.0097 (11)
N1	0.0743 (16)	0.097 (2)	0.079 (2)	−0.0081 (14)	0.0262 (14)	−0.0152 (16)
O1	0.153 (2)	0.0897 (17)	0.108 (2)	0.0012 (15)	0.0479 (17)	−0.0265 (14)
C4	0.0503 (13)	0.0654 (15)	0.0647 (17)	−0.0007 (11)	0.0197 (12)	−0.0018 (13)
C9	0.0637 (16)	0.0611 (16)	0.074 (2)	−0.0042 (12)	0.0232 (14)	0.0008 (14)
C5	0.0719 (17)	0.0616 (15)	0.0631 (17)	0.0063 (12)	0.0234 (14)	0.0069 (13)
C8	0.0521 (14)	0.0637 (15)	0.0671 (17)	−0.0018 (11)	0.0199 (12)	0.0027 (13)
C1	0.0543 (14)	0.0772 (18)	0.0669 (18)	−0.0048 (13)	0.0225 (13)	−0.0105 (14)
C2	0.0685 (17)	0.0858 (19)	0.0609 (17)	−0.0074 (15)	0.0234 (14)	0.0074 (15)
O2	0.165 (2)	0.133 (2)	0.0874 (18)	−0.0173 (17)	0.0648 (17)	−0.0174 (16)
C7	0.0620 (15)	0.0600 (15)	0.0683 (17)	0.0011 (12)	0.0228 (13)	0.0056 (13)
C3	0.0721 (17)	0.0674 (15)	0.0660 (17)	−0.0020 (13)	0.0263 (14)	0.0053 (14)
C6	0.0688 (17)	0.0653 (15)	0.0713 (18)	0.0054 (13)	0.0225 (14)	0.0017 (14)
C10	0.0645 (18)	0.0643 (18)	0.087 (2)	−0.0018 (13)	0.0157 (15)	0.0029 (15)
C12	0.107 (3)	0.0734 (19)	0.083 (2)	0.0020 (18)	0.023 (2)	−0.0097 (16)
C11	0.091 (2)	0.0665 (17)	0.094 (2)	−0.0030 (15)	0.0355 (18)	−0.0133 (16)
C13	0.083 (2)	0.107 (2)	0.103 (3)	−0.0017 (19)	0.025 (2)	−0.015 (2)
C14	0.088 (3)	0.196 (4)	0.128 (4)	−0.009 (3)	0.006 (2)	−0.038 (3)

Geometric parameters (Å, º)

S1—C8	1.744 (3)	C1—C2	1.374 (4)
S1—C10	1.774 (3)	C2—C3	1.371 (4)
O4—C9	1.208 (3)	C2—H2	0.9300
N2—C9	1.378 (3)	C7—H7	0.9300
N2—C10	1.384 (4)	C3—H3	0.9300
N2—C11	1.463 (3)	C6—H6	0.9300
O3—C10	1.202 (3)	C12—C13	1.506 (4)
N1—O1	1.207 (3)	C12—C11	1.516 (4)
N1—O2	1.223 (3)	C12—H12A	0.9700
N1—C1	1.466 (4)	C12—H12B	0.9700
C4—C5	1.394 (3)	C11—H11A	0.9700
C4—C3	1.402 (4)	C11—H11B	0.9700
C4—C7	1.461 (3)	C13—C14	1.511 (5)
C9—C8	1.490 (4)	C13—H13A	0.9700
C5—C6	1.373 (4)	C13—H13B	0.9700
C5—H5	0.9300	C14—H14A	0.9600
C8—C7	1.337 (3)	C14—H14B	0.9600
C1—C6	1.371 (4)	C14—H14C	0.9600
C8—S1—C10	91.56 (14)	C1—C6—C5	119.0 (3)
C9—N2—C10	115.3 (2)	C1—C6—H6	120.5
C9—N2—C11	121.9 (3)	C5—C6—H6	120.5
C10—N2—C11	122.7 (2)	O3—C10—N2	125.0 (3)
O1—N1—O2	122.6 (3)	O3—C10—S1	123.5 (3)
O1—N1—C1	118.8 (3)	N2—C10—S1	111.5 (2)
O2—N1—C1	118.6 (3)	C13—C12—C11	113.4 (3)
C5—C4—C3	117.8 (2)	C13—C12—H12A	108.9

C5—C4—C7	117.8 (2)	C11—C12—H12A	108.9
C3—C4—C7	124.4 (2)	C13—C12—H12B	108.9
O4—C9—N2	122.7 (3)	C11—C12—H12B	108.9
O4—C9—C8	125.7 (2)	H12A—C12—H12B	107.7
N2—C9—C8	111.6 (2)	N2—C11—C12	112.4 (2)
C6—C5—C4	121.3 (3)	N2—C11—H11A	109.1
C6—C5—H5	119.4	C12—C11—H11A	109.1
C4—C5—H5	119.4	N2—C11—H11B	109.1
C7—C8—C9	119.8 (2)	C12—C11—H11B	109.1
C7—C8—S1	130.2 (2)	H11A—C11—H11B	107.9
C9—C8—S1	110.06 (18)	C12—C13—C14	112.1 (3)
C6—C1—C2	121.9 (3)	C12—C13—H13A	109.2
C6—C1—N1	119.0 (3)	C14—C13—H13A	109.2
C2—C1—N1	119.1 (3)	C12—C13—H13B	109.2
C3—C2—C1	118.9 (3)	C14—C13—H13B	109.2
C3—C2—H2	120.5	H13A—C13—H13B	107.9
C1—C2—H2	120.5	C13—C14—H14A	109.5
C8—C7—C4	130.7 (2)	C13—C14—H14B	109.5
C8—C7—H7	114.7	H14A—C14—H14B	109.5
C4—C7—H7	114.7	C13—C14—H14C	109.5
C2—C3—C4	121.1 (2)	H14A—C14—H14C	109.5
C2—C3—H3	119.4	H14B—C14—H14C	109.5
C4—C3—H3	119.4		

C10—N2—C9—O4	−178.4 (3)	S1—C8—C7—C4	−1.2 (4)
C11—N2—C9—O4	0.0 (4)	C5—C4—C7—C8	178.7 (2)
C10—N2—C9—C8	0.6 (3)	C3—C4—C7—C8	−1.8 (4)
C11—N2—C9—C8	179.0 (2)	C1—C2—C3—C4	0.5 (4)
C3—C4—C5—C6	−0.2 (4)	C5—C4—C3—C2	−0.4 (4)
C7—C4—C5—C6	179.3 (2)	C7—C4—C3—C2	−179.9 (2)
O4—C9—C8—C7	−0.5 (4)	C2—C1—C6—C5	−0.6 (4)
N2—C9—C8—C7	−179.6 (2)	N1—C1—C6—C5	179.3 (2)
O4—C9—C8—S1	178.5 (2)	C4—C5—C6—C1	0.7 (4)
N2—C9—C8—S1	−0.5 (3)	C9—N2—C10—O3	179.0 (3)
C10—S1—C8—C7	179.1 (3)	C11—N2—C10—O3	0.6 (4)
C10—S1—C8—C9	0.19 (18)	C9—N2—C10—S1	−0.5 (3)
O1—N1—C1—C6	7.1 (4)	C11—N2—C10—S1	−178.87 (19)
O2—N1—C1—C6	−173.9 (3)	C8—S1—C10—O3	−179.3 (3)
O1—N1—C1—C2	−173.0 (3)	C8—S1—C10—N2	0.1 (2)
O2—N1—C1—C2	6.0 (4)	C9—N2—C11—C12	79.0 (3)
C6—C1—C2—C3	0.1 (4)	C10—N2—C11—C12	−102.8 (3)
N1—C1—C2—C3	−179.8 (2)	C13—C12—C11—N2	70.2 (3)
C9—C8—C7—C4	177.6 (2)	C11—C12—C13—C14	−175.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···S1	0.93	2.55	3.256 (3)	133

C2—H2···O4^{i}	0.93	2.45	3.139 (4)	131
C5—H5···O2^{ii}	0.93	2.60	3.468 (4)	156
C11—H11*B*···O3^{iii}	0.97	2.60	3.281 (3)	128

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