N,N-Diethyl-2-[5-(4-methoxybenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl]acetamide

Vijayan Viswanathan,[a] Sabina Yasmin,[b] Venkatesan Jayaprakash[b] and Devadasan Velmurugan[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Pharmaceutical Sciences & Technology, Birla Institute of Technology, Mesra, Ranchi 835 215, Jharkhand, India. *Correspondence e-mail: shirai2011@gmail.com

In the title compound, $C_{17}H_{20}N_2O_4S$, the thiazolidine (r.m.s. deviation = 0.022 Å) and phenyl rings (major and minor occupancies) are inclined to one another by 6.3 (3) and 10.5 (3)°, respectively. The molecular conformation is stabilized by an intramolecular C—H···S interaction. In the crystal, molecules are linked by C—H···O hydrogen bonds, which generate $R_2^2(18)$, $R_2^2(24)$ and $R_2^1(7)$ ring motifs. Aromatic π–π stacking interactions are also observed.

3D view
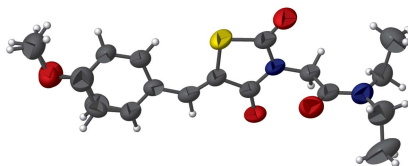
Chemical scheme
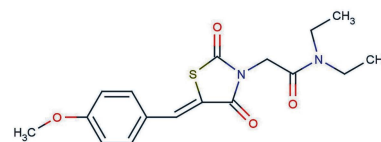
Structure description

Thiazolidine-2,4-dione derivatives show a number of biological properties including anticancer, antiarthritic, anti-inflammatory, anti-oxidant and diabetes related effects (Fujita et al., 1983; Youssef et al., 2010; Albrecht et al., 2005). As part of our investigations of thiazolidine derivatives, we have undertaken the X-ray crystal structure analysis of the title compound.

The molecular structure of the compound is shown in Fig. 1. The thiazolidine ring adopts its expected planar conformation with a maximum deviation of 0.0266 (4) Å for C11. The methoxy group and atoms C2 and C7 of the phenyl ring are disordered over two orientations with site occupancy factors of 0.579 (15):0.421 (15). The mean planes of the thiazolidine and phenyl rings (major and minor occupancies) are inclined to one another by 6.3 (3) and 10.5 (3)°, respectively. The 2-aminoacetamide moiety is in an extended conformation, as can be seen from the N1—C12—C13—N2 torsion angle of −166.4 (3)°. The torsion angles of the diethylamine group are C13—N2—C16—C17 = 83.3 (5)° and C13—N2—C14—C15 = 90.8 (4)°. An intramolecular C—H···S contact (Table 1) generates an S(6) ring.
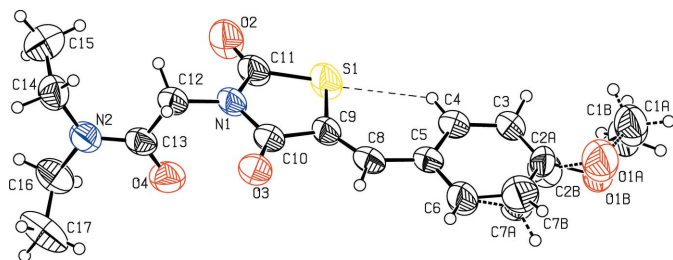
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Figure 1
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$\cdots$S1	0.93	2.56	3.259 (4)	133
C1B—H1B3$\cdots$O2^{i}	0.96	2.51	3.160 (14)	125
C3—H3$\cdots$O2^{i}	0.93	2.58	3.481 (5)	164
C12—H12$B\cdots$O3^{ii}	0.97	2.43	3.342 (4)	157

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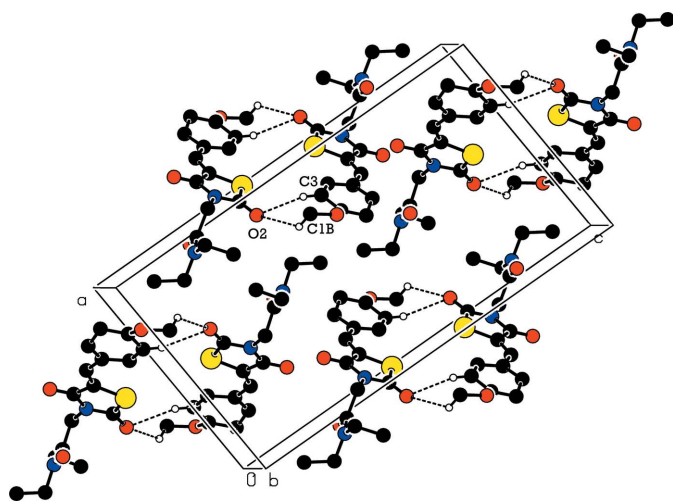

Figure 2
The C—H$\cdots$O intermolecular interactions generating $R_2^2(14)$ and $R_2^2(24)$ ring motifs, viewed along the b axis. H atoms not involved in hydrogen bonds have been excluded for clarity.
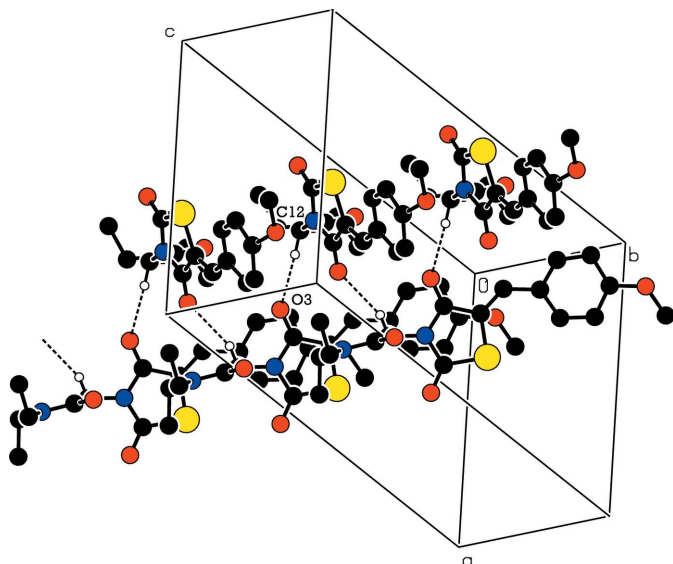
Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{20}N_2O_4S$
M_r	348.41
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	11.6978 (6), 7.1331 (4), 21.1822 (12)
β (°)	95.311 (4)
V (Å^3)	1759.89 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.28 × 0.23 × 0.17
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.752, 0.863
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12523, 4146, 1342
R_{int}	0.053
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.212, 0.84
No. of reflections	4146
No. of parameters	258
No. of restraints	56
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.17, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2016* (Sheldrick, 2015).
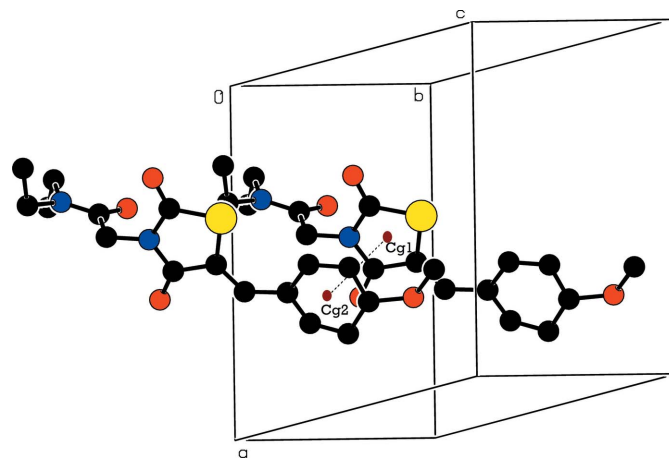

Figure 3
The C12—H12$B\cdots$O3 intermolecular hydrogen bond generates $C(5)$ zigzag chains.

Figure 4
The weak π–π interaction of the title compound, viewed along the c axis.

In the crystal, the C3—H3···O2 interaction generates an $R_2^2(18)$ loop and the C1B—H13B···O2 hydrogen bond leads to an $R_2^2(24)$ loop (Fig. 2). The C12—H12B···O3 hydrogen bond generates a $C(5)$ zigzag chain running along [101], as shown in Fig. 3. Aromatic π–π stacking interactions are observed, as shown in Fig. 4, with a $Cg1···Cg2(x, -1 + y, z)$ distance of 3.879 (3) Å where $Cg1$ and $Cg2$ are the centroids of the thiazolidine and phenyl rings, respectively.

Synthesis and crystallization

To a stirred solution of *p*-methoxybenzylidine thiazolidinedione (0.5 g; 2.2 mmol) in 25 ml of acetonitrile was added 2-chloro-*N*,*N*-diethylacetamide (0.3 g; 2.4 mmol) and the mixture was refluxed for 16 h and cooled to room temperature. The reaction mixture was then poured into ice-cooled water. The crude brown-colored solid that separated was filtered and dried to give the title compound as a crystalline powder (yield = 82%). After purification, the compound was recrystallized from $CHCl_3$ solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methoxy group and atoms C2/C7 of the phenyl ring are disordered over two orientations with site occupancy factors of 0.579 (15):0.421 (15).

References

Albrecht, U., Gördes, D., Schmidt, E., Thurow, K., Lalk, M. & Langer, P. (2005). *Bioorg. Med. Chem.* **13**, 4402–4407.
Bruker (2008). *APEX2, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fujita, T., Sugiyama, Y., Taketomi, S., Sohda, T., Kawamatsu, Y., Iwatsuka, H. & Suzuoki, Z. (1983). *Diabetes*, **32**, 804–810.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Youssef, A. M., Sydney White, M., Villanueva, E. B., El-Ashmawy, I. M. & Klegeris, A. (2010). *Bioorg. Med. Chem.* **18**, 2019–2028.

full crystallographic data

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N,N-Diethyl-2-[5-(4-methoxybenzylidene)-2,4-dioxo-1,3-thiazolidin-3-yl]acetamide

Crystal data

$C_{17}H_{20}N_2O_4S$	$F(000) = 736$
$M_r = 348.41$	$D_x = 1.315$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.6978$ (6) Å	Cell parameters from 4146 reflections
$b = 7.1331$ (4) Å	$\theta = 1.9$–28.0°
$c = 21.1822$ (12) Å	$\mu = 0.21$ mm^{-1}
$\beta = 95.311$ (4)°	$T = 293$ K
$V = 1759.89$ (17) Å^3	Block, brown
$Z = 4$	$0.28 \times 0.23 \times 0.17$ mm

Data collection

Bruker SMART APEXII CCD diffractometer	4146 independent reflections
	1342 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.053$
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)	$\theta_{max} = 28.0°$, $\theta_{min} = 1.9°$
	$h = -15 \rightarrow 11$
$T_{min} = 0.752$, $T_{max} = 0.863$	$k = -9 \rightarrow 9$
12523 measured reflections	$l = -27 \rightarrow 24$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.212$	$w = 1/[\sigma^2(F_o^2) + (0.1074P)^2]$
$S = 0.84$	where $P = (F_o^2 + 2F_c^2)/3$
4146 reflections	$(\Delta/\sigma)_{max} < 0.001$
258 parameters	$\Delta\rho_{max} = 0.17$ e Å^{-3}
56 restraints	$\Delta\rho_{min} = -0.19$ 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. The H atoms were placed in calculated positions with C—H = 0.93 Å to 0.97 Å, refined in the riding model with fixed isotropic displacement parameters: $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl group and $U_{iso}(H) = 1.2U_{eq}(C)$ for other groups.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C3	0.6852 (4)	0.3920 (6)	0.98139 (18)	0.0889 (12)	
H3	0.645923	0.404422	1.017386	0.107*	
C4	0.6695 (3)	0.2315 (6)	0.94622 (18)	0.0798 (11)	
H4	0.608647	0.153121	0.953630	0.096*	
C5	0.7400 (3)	0.1804 (5)	0.90020 (17)	0.0692 (10)	
C6	0.8256 (4)	0.3040 (7)	0.8900 (2)	0.1029 (14)	
H6	0.885074	0.269085	0.866210	0.124*	
C8	0.7292 (3)	0.0126 (6)	0.86181 (16)	0.0716 (10)	
H8	0.787318	−0.003383	0.835153	0.086*	
C9	0.6511 (3)	−0.1225 (5)	0.85793 (16)	0.0693 (10)	
C10	0.6611 (3)	−0.2856 (5)	0.81545 (17)	0.0713 (10)	
C11	0.4918 (4)	−0.3558 (6)	0.86037 (18)	0.0849 (12)	
C12	0.5567 (3)	−0.5782 (5)	0.78347 (16)	0.0690 (10)	
H12A	0.521585	−0.674578	0.807565	0.083*	
H12B	0.630996	−0.623818	0.773382	0.083*	
C13	0.4810 (3)	−0.5400 (7)	0.72212 (18)	0.0680 (10)	
C14	0.4522 (3)	−0.8817 (5)	0.71029 (19)	0.0840 (11)	
H14A	0.523234	−0.894418	0.737439	0.101*	
H14B	0.457094	−0.962399	0.673789	0.101*	
C15	0.3535 (4)	−0.9451 (6)	0.7461 (2)	0.1128 (15)	
H15A	0.353226	−0.874479	0.784671	0.169*	
H15B	0.361974	−1.076036	0.756010	0.169*	
H15C	0.282503	−0.925314	0.720459	0.169*	
C16	0.3669 (4)	−0.6514 (6)	0.6298 (2)	0.1011 (14)	
H16A	0.318532	−0.543771	0.635958	0.121*	
H16B	0.317224	−0.758599	0.620371	0.121*	
C17	0.4347 (5)	−0.6150 (9)	0.5744 (2)	0.139 (2)	
H17A	0.483720	−0.508536	0.583319	0.209*	
H17B	0.383143	−0.590304	0.537429	0.209*	
H17C	0.480638	−0.722981	0.567051	0.209*	
N1	0.5719 (2)	−0.4109 (4)	0.82111 (13)	0.0699 (8)	
N2	0.4399 (3)	−0.6879 (5)	0.68896 (15)	0.0787 (9)	
O2	0.4063 (3)	−0.4452 (4)	0.86787 (13)	0.1112 (10)	
O3	0.7349 (2)	−0.3119 (3)	0.78051 (12)	0.0892 (9)	
O4	0.4629 (2)	−0.3782 (4)	0.70499 (12)	0.0911 (8)	
S1	0.52785 (9)	−0.14350 (16)	0.89820 (5)	0.0943 (5)	
O1A	0.8368 (13)	0.629 (2)	1.0134 (6)	0.130 (5)	0.416 (16)
C1A	0.7701 (18)	0.694 (3)	1.0625 (9)	0.115 (6)	0.416 (16)
H1A1	0.708181	0.770687	1.044279	0.173*	0.416 (16)
H1A2	0.817939	0.765989	1.092696	0.173*	0.416 (16)
H1A3	0.739503	0.588108	1.083304	0.173*	0.416 (16)
C7A	0.8220 (12)	0.4863 (13)	0.9161 (6)	0.065 (4)	0.416 (16)
H7A	0.865855	0.579302	0.899298	0.078*	0.416 (16)
C2A	0.7561 (12)	0.536 (2)	0.9662 (7)	0.100 (7)	0.416 (16)
C2B	0.7809 (10)	0.4968 (13)	0.9732 (6)	0.093 (5)	0.584 (16)

C1B	0.7046 (13)	0.7394 (19)	1.0444 (6)	0.113 (4)	0.584 (16)
H1B1	0.625442	0.717329	1.030028	0.170*	0.584 (16)
H1B2	0.715029	0.869088	1.055557	0.170*	0.584 (16)
H1B3	0.726055	0.662618	1.080745	0.170*	0.584 (16)
C7B	0.8638 (11)	0.4416 (18)	0.9326 (6)	0.118 (5)	0.584 (16)
H7B	0.937125	0.492941	0.934397	0.142*	0.584 (16)
O1B	0.7743 (8)	0.6939 (9)	0.9952 (4)	0.093 (3)	0.584 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.129 (3)	0.086 (3)	0.056 (3)	−0.022 (3)	0.027 (2)	−0.011 (2)
C4	0.100 (3)	0.082 (3)	0.060 (2)	−0.014 (2)	0.025 (2)	−0.003 (2)
C5	0.082 (2)	0.079 (3)	0.049 (2)	−0.010 (2)	0.0145 (19)	0.002 (2)
C6	0.124 (3)	0.114 (4)	0.077 (3)	−0.041 (3)	0.044 (3)	−0.027 (3)
C8	0.081 (2)	0.087 (3)	0.049 (2)	0.002 (2)	0.0207 (18)	0.000 (2)
C9	0.078 (2)	0.079 (3)	0.054 (2)	−0.009 (2)	0.0191 (18)	−0.009 (2)
C10	0.082 (3)	0.080 (3)	0.055 (2)	−0.004 (2)	0.023 (2)	−0.003 (2)
C11	0.088 (3)	0.108 (3)	0.063 (3)	−0.019 (2)	0.034 (2)	−0.015 (2)
C12	0.076 (2)	0.077 (3)	0.056 (2)	−0.0049 (18)	0.0196 (19)	−0.003 (2)
C13	0.074 (2)	0.076 (3)	0.056 (3)	0.008 (2)	0.020 (2)	0.001 (2)
C14	0.094 (3)	0.077 (3)	0.080 (3)	0.006 (2)	0.004 (2)	−0.012 (2)
C15	0.109 (3)	0.103 (3)	0.127 (4)	−0.008 (3)	0.016 (3)	0.016 (3)
C16	0.104 (3)	0.127 (4)	0.069 (3)	0.008 (3)	−0.012 (3)	0.006 (3)
C17	0.144 (4)	0.213 (6)	0.060 (3)	0.053 (4)	0.012 (3)	−0.006 (3)
N1	0.0775 (19)	0.085 (2)	0.0514 (18)	−0.0103 (17)	0.0247 (15)	−0.0113 (17)
N2	0.093 (2)	0.082 (2)	0.061 (2)	0.0030 (18)	0.0035 (17)	0.0002 (19)
O2	0.0970 (19)	0.143 (3)	0.102 (2)	−0.0388 (19)	0.0535 (17)	−0.0404 (19)
O3	0.0999 (18)	0.098 (2)	0.0784 (19)	−0.0146 (14)	0.0527 (15)	−0.0159 (14)
O4	0.118 (2)	0.0776 (19)	0.079 (2)	0.0135 (15)	0.0182 (15)	0.0101 (16)
S1	0.0933 (8)	0.1155 (9)	0.0805 (8)	−0.0162 (6)	0.0426 (6)	−0.0324 (7)
O1A	0.139 (8)	0.135 (8)	0.122 (8)	−0.032 (6)	0.038 (6)	−0.031 (6)
C1A	0.116 (12)	0.127 (12)	0.107 (12)	−0.022 (9)	0.032 (10)	−0.038 (9)
C7A	0.060 (6)	0.075 (7)	0.062 (6)	−0.010 (5)	0.014 (5)	0.009 (5)
C2A	0.110 (9)	0.102 (11)	0.085 (10)	−0.004 (7)	−0.005 (7)	−0.002 (8)
C2B	0.143 (8)	0.070 (6)	0.073 (7)	−0.042 (6)	0.042 (6)	−0.026 (5)
C1B	0.143 (10)	0.105 (7)	0.093 (7)	−0.016 (7)	0.012 (8)	−0.026 (6)
C7B	0.120 (8)	0.136 (8)	0.102 (7)	−0.039 (6)	0.029 (6)	−0.012 (6)
O1B	0.120 (6)	0.081 (4)	0.081 (4)	−0.021 (3)	0.027 (4)	−0.016 (3)

Geometric parameters (Å, º)

C3—C4	1.369 (5)	C14—C15	1.509 (5)
C3—C2B	1.371 (7)	C14—H14A	0.9700
C3—C2A	1.377 (9)	C14—H14B	0.9700
C3—H3	0.9300	C15—H15A	0.9600
C4—C5	1.383 (5)	C15—H15B	0.9600
C4—H4	0.9300	C15—H15C	0.9600

C5—C6	1.366 (5)	C16—N2	1.472 (4)
C5—C8	1.446 (5)	C16—C17	1.498 (6)
C6—C7B	1.380 (8)	C16—H16A	0.9700
C6—C7A	1.415 (8)	C16—H16B	0.9700
C6—H6	0.9300	C17—H17A	0.9600
C8—C9	1.325 (4)	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600
C9—C10	1.482 (5)	O1A—C2A	1.469 (9)
C9—S1	1.748 (4)	O1A—C1A	1.432 (19)
C10—O3	1.203 (4)	C1A—H1A1	0.9600
C10—N1	1.387 (4)	C1A—H1A2	0.9600
C11—O2	1.210 (4)	C1A—H1A3	0.9600
C11—N1	1.367 (4)	C7A—C2A	1.413 (9)
C11—S1	1.746 (4)	C7A—H7A	0.9300
C12—N1	1.437 (4)	C2B—C7B	1.410 (8)
C12—C13	1.528 (5)	C2B—O1B	1.486 (9)
C12—H12A	0.9700	C1B—O1B	1.418 (14)
C12—H12B	0.9700	C1B—H1B1	0.9600
C13—O4	1.222 (4)	C1B—H1B2	0.9600
C13—N2	1.332 (4)	C1B—H1B3	0.9600
C14—N2	1.457 (4)	C7B—H7B	0.9300
C4—C3—C2B	117.2 (5)	H15B—C15—H15C	109.5
C4—C3—C2A	123.4 (7)	N2—C16—C17	112.9 (4)
C4—C3—H3	118.3	N2—C16—H16A	109.0
C2A—C3—H3	118.3	C17—C16—H16A	109.0
C3—C4—C5	123.1 (4)	N2—C16—H16B	109.0
C3—C4—H4	118.5	C17—C16—H16B	109.0
C5—C4—H4	118.5	H16A—C16—H16B	107.8
C6—C5—C4	115.8 (4)	C16—C17—H17A	109.5
C6—C5—C8	118.2 (3)	C16—C17—H17B	109.5
C4—C5—C8	126.0 (3)	H17A—C17—H17B	109.5
C5—C6—C7B	123.6 (6)	C16—C17—H17C	109.5
C5—C6—C7A	118.8 (6)	H17A—C17—H17C	109.5
C5—C6—H6	120.6	H17B—C17—H17C	109.5
C7A—C6—H6	120.6	C11—N1—C10	115.5 (3)
C9—C8—C5	131.4 (3)	C11—N1—C12	121.3 (3)
C9—C8—H8	114.3	C10—N1—C12	122.8 (3)
C5—C8—H8	114.3	C13—N2—C14	124.6 (3)
C8—C9—C10	121.0 (3)	C13—N2—C16	117.4 (3)
C8—C9—S1	128.8 (3)	C14—N2—C16	117.7 (3)
C10—C9—S1	110.1 (3)	C11—S1—C9	91.45 (19)
O3—C10—N1	122.8 (3)	C2A—O1A—C1A	106.3 (11)
O3—C10—C9	126.7 (3)	O1A—C1A—H1A1	109.5
N1—C10—C9	110.5 (3)	O1A—C1A—H1A2	109.5
O2—C11—N1	123.4 (4)	H1A1—C1A—H1A2	109.5
O2—C11—S1	124.4 (3)	O1A—C1A—H1A3	109.5
N1—C11—S1	112.3 (3)	H1A1—C1A—H1A3	109.5

N1—C12—C13	110.9 (3)	H1A2—C1A—H1A3	109.5
N1—C12—H12A	109.5	C2A—C7A—C6	124.3 (11)
C13—C12—H12A	109.5	C2A—C7A—H7A	117.9
N1—C12—H12B	109.5	C6—C7A—H7A	117.9
C13—C12—H12B	109.5	C3—C2A—C7A	111.7 (12)
H12A—C12—H12B	108.1	C3—C2A—O1A	122.9 (12)
O4—C13—N2	123.2 (4)	C7A—C2A—O1A	105.3 (10)
O4—C13—C12	119.4 (4)	C3—C2B—C7B	122.8 (7)
N2—C13—C12	117.3 (3)	C3—C2B—O1B	114.1 (8)
N2—C14—C15	112.5 (3)	C7B—C2B—O1B	121.0 (7)
N2—C14—H14A	109.1	O1B—C1B—H1B1	109.5
C15—C14—H14A	109.1	O1B—C1B—H1B2	109.5
N2—C14—H14B	109.1	H1B1—C1B—H1B2	109.5
C15—C14—H14B	109.1	O1B—C1B—H1B3	109.5
H14A—C14—H14B	107.8	H1B1—C1B—H1B3	109.5
C14—C15—H15A	109.5	H1B2—C1B—H1B3	109.5
C14—C15—H15B	109.5	C6—C7B—C2B	113.4 (8)
H15A—C15—H15B	109.5	C6—C7B—H7B	123.3
C14—C15—H15C	109.5	C2B—C7B—H7B	123.3
H15A—C15—H15C	109.5	C1B—O1B—C2B	119.8 (8)
C2B—C3—C4—C5	−5.2 (9)	C13—C12—N1—C10	−90.0 (4)
C2A—C3—C4—C5	13.9 (11)	O4—C13—N2—C14	−175.0 (3)
C3—C4—C5—C6	−2.1 (6)	C12—C13—N2—C14	6.7 (5)
C3—C4—C5—C8	179.4 (4)	O4—C13—N2—C16	−1.7 (5)
C4—C5—C6—C7B	18.5 (11)	C12—C13—N2—C16	−180.0 (3)
C8—C5—C6—C7B	−162.8 (9)	C15—C14—N2—C13	90.8 (4)
C4—C5—C6—C7A	−12.8 (8)	C15—C14—N2—C16	−82.5 (4)
C8—C5—C6—C7A	165.8 (7)	C17—C16—N2—C13	83.3 (5)
C6—C5—C8—C9	−174.3 (4)	C17—C16—N2—C14	−102.9 (4)
C4—C5—C8—C9	4.1 (6)	O2—C11—S1—C9	−178.0 (4)
C5—C8—C9—C10	−178.2 (3)	N1—C11—S1—C9	2.3 (3)
C5—C8—C9—S1	1.4 (6)	C8—C9—S1—C11	−179.9 (4)
C8—C9—C10—O3	−1.7 (6)	C10—C9—S1—C11	−0.3 (3)
S1—C9—C10—O3	178.6 (3)	C5—C6—C7A—C2A	18.5 (17)
C8—C9—C10—N1	177.9 (3)	C4—C3—C2A—C7A	−8.5 (18)
S1—C9—C10—N1	−1.7 (4)	C4—C3—C2A—O1A	−135.0 (14)
N1—C12—C13—O4	15.3 (4)	C6—C7A—C2A—C3	−7 (2)
N1—C12—C13—N2	−166.4 (3)	C6—C7A—C2A—O1A	128.3 (16)
O2—C11—N1—C10	176.3 (4)	C1A—O1A—C2A—C3	−55 (2)
S1—C11—N1—C10	−3.9 (4)	C1A—O1A—C2A—C7A	175.7 (13)
O2—C11—N1—C12	2.7 (6)	C4—C3—C2B—C7B	−2.6 (16)
S1—C11—N1—C12	−177.5 (3)	C4—C3—C2B—O1B	161.0 (8)
O3—C10—N1—C11	−176.7 (3)	C5—C6—C7B—C2B	−25.2 (16)
C9—C10—N1—C11	3.6 (4)	C3—C2B—C7B—C6	16.7 (18)
O3—C10—N1—C12	−3.2 (5)	O1B—C2B—C7B—C6	−145.8 (15)
C9—C10—N1—C12	177.2 (3)	C3—C2B—O1B—C1B	27.2 (16)
C13—C12—N1—C11	83.2 (4)	C7B—C2B—O1B—C1B	−168.9 (11)

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C4—H4⋯S1	0.93	2.56	3.259 (4)	133
C1*B*—H1*B*3⋯O2^{i}	0.96	2.51	3.160 (14)	125
C3—H3⋯O2^{i}	0.93	2.58	3.481 (5)	164
C12—H12*B*⋯O3^{ii}	0.97	2.43	3.342 (4)	157

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