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(5*Z*)-3-(2-Oxopropyl)-5-(3,4,5-trimethoxybenzylidene)-1,3-thiazolidine-2,4-dione

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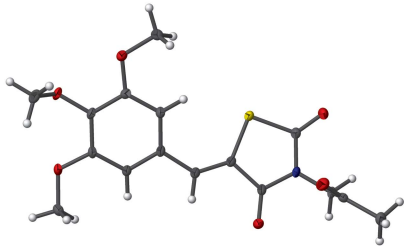
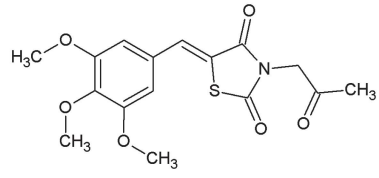
In the crystal of the title molecule, $C_{16}H_{17}NO_6S$, there are three sets of intermolecular C—H···O hydrogen bonds, as well as two sets of intermolecular C—H···π(ring) interactions. In addition, the thiazolidene rings participate in offset π–π stacking interactions [centroid–centroid distance = 3.685 (1) Å]. These generate small channels running parallel to the *a* axis with approximate cross-sections of 3.7 × 8.1 Å.

3D view



Chemical scheme



Structure description

Thiazolidine-2,4-dione scaffold compounds are considered to be an important class of heterocycles due to their diverse biological activities. They have been reported to exhibit anti-cancer (Ashok & Vanaja, 2016; Wei *et al.*, 2009; Xia *et al.*, 2009), anti-plasmodial inhibitor (Sharma *et al.*, 2015), anti-leishmanial (Leite *et al.*, 2016), anti-inflammatory (Barros *et al.*, 2010), anti-microbial (Liu *et al.*, 2011), anti-oxidant and anti-hyperglycemic activities (Koppireddi *et al.*, 2013; Oakes *et al.*, 1994). In this context, we report herein the synthesis and crystal structure of the title compound.

In the title molecule (Fig. 1), the dihedral angle between the five- and six-membered ring is 17.67 (7)°. In the crystal, there are small channels of approximately 3.7 *x* 8.1 Å running parallel to the *a* axis (Fig. 2). In addition to the three sets of C—H···O hydrogen bonds (Table 1 and Figs. 2 and 3), there is an offset π–π stacking interaction between the

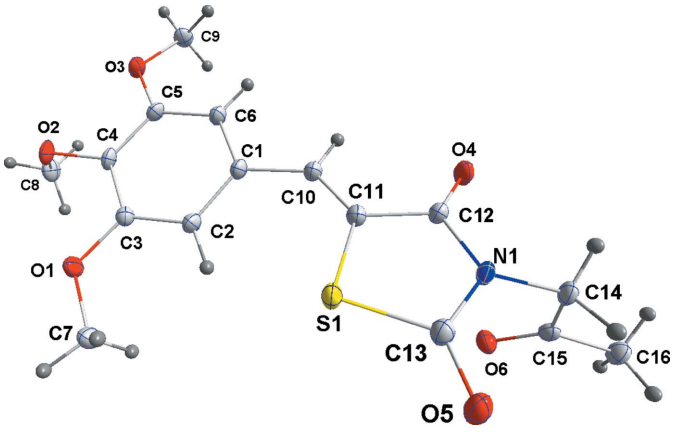


Figure 1
The title molecule, showing the atom-labeling scheme and 50% probability ellipsoids.

thiazolidene ring and its counterpart at $1 - x$, $1 - y$, $-z$ [centroid–centroid distance = 3.6854 (7) Å] and two intermolecular C—H···π(ring) interactions (Table 1).

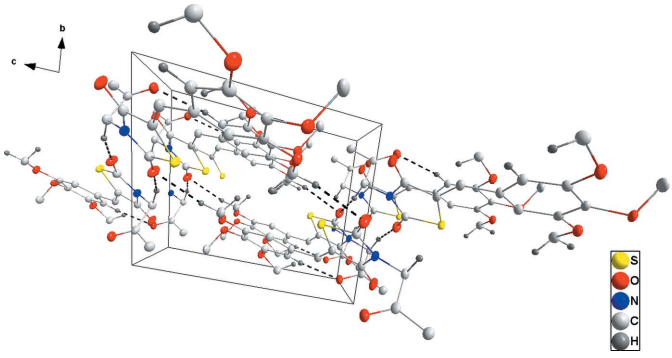


Figure 2
Packing viewed along the *a* axis with C—H···O hydrogen bonds shown as dotted lines.

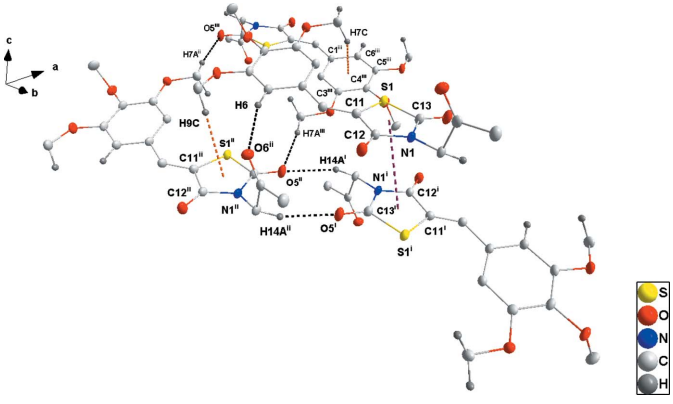


Figure 3
Detail of the intermolecular interactions: offset π-stacking (purple dotted line); C—H···π(ring) (orange dotted lines); C—H···O (black dotted lines) [symmetry codes: (i) $1 - x, 1 - y, -z$; (ii) $-1 + x, y, z$; (iii) $-x, 1 - y, 1 - z$].

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and S1/N1/C11–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O6^{i}	0.942 (14)	2.398 (14)	3.3108 (14)	163.2 (12)
C7—H7*A*···O5^{ii}	0.971 (15)	2.482 (15)	3.4434 (15)	170.4 (13)
C14—H14*A*···O5^{iii}	1.016 (15)	2.335 (15)	3.2659 (14)	151.8 (11)
C7—H7*C*···*Cg*1^{iv}	0.994 (15)	2.755 (15)	3.5131 (14)	133.3 (11)
C9—H9*C*···*Cg*2^{i}	1.001 (14)	2.900 (15)	3.8441 (14)	157.5 (11)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}NO_6S$
M_r	351.36
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	7.2771 (5), 9.9612 (7), 11.9257 (8)
α, β, γ (°)	78.778 (1), 75.616 (1), 72.829 (1)
V (Å^3)	793.16 (9)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.24
Crystal size (mm)	0.33 × 0.22 × 0.21
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.88, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15337, 4235, 3660
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.111, 1.12
No. of reflections	4235
No. of parameters	285
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.24

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

A mixture of 5-(3,4,5-trimethoxybenzylidene)-1,3-thiazolidine-2,4-dione potassium salt (10 mmol, 3.33 g) and chloroacetone (11 mmol, 1.02 g, 0.91 mL), in DMF (10 mL) was heated under gentle reflux for 8 h. The reaction mixture was cooled to room temperature and the resulting precipitate was filtered off, washed with water and recrystallized from ethanol and a few drops of dioxane to give good quality crystals suitable for X-ray diffraction (m.p. 411–413 K, 86% yield).

^{1}H NMR (300 MHz, DMSO-d_6): *d* 2.52 (*s*, 3H), 3.74 (*s*, 3H), 3.84 (*s*, 6H), 4.68 (*s*, 2H), 6.96 (*s*, 2H), 7.92 (*s*, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): *d* 27.5, 50.7, 56.5, 60.6, 108.1, 120.2, 128.7, 134.3, 140.1, 153.7 165.4, 167.2, and 200.8. *m*/*z* = 352 $[M + H]^+$.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161959 [https://doi.org/10.1107/S2414314616019593]

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Crystal data

$C_{16}H_{17}NO_6S$
M_r = 351.36
Triclinic, $P\overline{1}$
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b = 9.9612 (7) Å
c = 11.9257 (8) Å
α = 78.778 (1)°
β = 75.616 (1)°
γ = 72.829 (1)°
V = 793.16 (9) Å^3
Z = 2
$F(000)$ = 368
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9211 reflections
θ = 2.6–29.3°
μ = 0.24 mm^{-1}
T = 100 K
Block, colourless
0.33 × 0.22 × 0.21 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.88, T_{max} = 0.95
15337 measured reflections
4235 independent reflections
3660 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 29.3°, θ_{min} = 1.8°
h = −10→9
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.12
4235 reflections
285 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.0197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 15 sec/frame.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
S1	0.48040 (4)	0.43973 (3)	0.23681 (2)	0.01742 (10)
O1	0.03935 (12)	0.33614 (9)	0.63528 (7)	0.01876 (18)
O2	−0.28654 (12)	0.25762 (9)	0.64722 (7)	0.01887 (18)
O3	−0.33832 (11)	0.15463 (9)	0.46574 (7)	0.01978 (19)
O4	0.52749 (13)	0.21005 (10)	0.00080 (7)	0.0234 (2)
O5	0.80964 (14)	0.50044 (10)	0.11411 (8)	0.0261 (2)
O6	0.97444 (13)	0.12856 (9)	0.08413 (7)	0.02220 (19)
N1	0.68693 (13)	0.35869 (10)	0.03734 (8)	0.0158 (2)
C1	0.12221 (16)	0.26129 (12)	0.33290 (9)	0.0155 (2)
C2	0.15413 (16)	0.30468 (12)	0.42980 (9)	0.0161 (2)
H2	0.270 (2)	0.3321 (17)	0.4249 (14)	0.030 (4)*
C3	0.02037 (16)	0.29904 (11)	0.53540 (9)	0.0149 (2)
C4	−0.14759 (16)	0.25128 (11)	0.54493 (9)	0.0153 (2)
C5	−0.17503 (16)	0.20396 (12)	0.44871 (10)	0.0158 (2)
C6	−0.04092 (16)	0.20892 (12)	0.34351 (10)	0.0159 (2)
H6	−0.058 (2)	0.1776 (14)	0.2782 (13)	0.021 (4)*
C7	0.21364 (18)	0.38004 (13)	0.62923 (10)	0.0199 (2)
H7A	0.203 (2)	0.4033 (16)	0.7063 (13)	0.027 (4)*
H7B	0.328 (2)	0.2998 (15)	0.6124 (13)	0.022 (4)*
H7C	0.218 (2)	0.4641 (15)	0.5688 (13)	0.020 (3)*
C8	−0.2732 (2)	0.12561 (14)	0.72236 (11)	0.0234 (3)
H8A	−0.297 (2)	0.0581 (17)	0.6826 (14)	0.030 (4)*
H8B	−0.382 (2)	0.1412 (16)	0.7911 (14)	0.029 (4)*
H8C	−0.145 (3)	0.0923 (17)	0.7438 (14)	0.034 (4)*
C9	−0.33885 (18)	0.07211 (13)	0.38013 (11)	0.0201 (2)
H9A	−0.228 (2)	−0.0124 (15)	0.3783 (12)	0.022 (4)*
H9B	−0.462 (2)	0.0468 (14)	0.4033 (12)	0.017 (3)*

H9C	−0.333 (2)	0.1296 (15)	0.3011 (13)	0.022 (4)*
C10	0.25748 (16)	0.25979 (12)	0.21977 (10)	0.0166 (2)
H10	0.239 (2)	0.2061 (14)	0.1678 (12)	0.017 (3)*
C11	0.40602 (16)	0.32201 (12)	0.17634 (9)	0.0157 (2)
C12	0.53935 (16)	0.28850 (12)	0.06331 (9)	0.0160 (2)
C13	0.68703 (17)	0.43854 (12)	0.12030 (10)	0.0177 (2)
C14	0.85791 (16)	0.32219 (12)	−0.05548 (10)	0.0166 (2)
H14A	0.922 (2)	0.4040 (16)	−0.0822 (13)	0.024 (4)*
H14B	0.819 (2)	0.3053 (15)	−0.1204 (13)	0.020 (3)*
C15	1.00626 (16)	0.18907 (12)	−0.01512 (9)	0.0162 (2)
C16	1.19038 (18)	0.14177 (14)	−0.10274 (11)	0.0206 (2)
H16A	1.154 (2)	0.1391 (18)	−0.1711 (15)	0.037 (4)*
H16B	1.270 (2)	0.0529 (17)	−0.0750 (14)	0.025 (4)*
H16C	1.254 (3)	0.2144 (19)	−0.1146 (16)	0.045 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01803 (16)	0.02014 (16)	0.01488 (15)	−0.00891 (11)	0.00277 (11)	−0.00591 (11)
O1	0.0189 (4)	0.0252 (4)	0.0137 (4)	−0.0090 (3)	−0.0002 (3)	−0.0052 (3)
O2	0.0161 (4)	0.0196 (4)	0.0167 (4)	−0.0048 (3)	0.0070 (3)	−0.0055 (3)
O3	0.0143 (4)	0.0281 (4)	0.0190 (4)	−0.0113 (3)	0.0031 (3)	−0.0072 (3)
O4	0.0235 (4)	0.0344 (5)	0.0172 (4)	−0.0160 (4)	0.0027 (3)	−0.0105 (3)
O5	0.0280 (5)	0.0328 (5)	0.0228 (4)	−0.0206 (4)	0.0054 (4)	−0.0099 (4)
O6	0.0254 (5)	0.0255 (4)	0.0154 (4)	−0.0080 (4)	−0.0023 (3)	−0.0022 (3)
N1	0.0134 (4)	0.0203 (5)	0.0133 (4)	−0.0073 (4)	0.0027 (3)	−0.0039 (3)
C1	0.0135 (5)	0.0184 (5)	0.0136 (5)	−0.0058 (4)	0.0004 (4)	−0.0014 (4)
C2	0.0136 (5)	0.0196 (5)	0.0154 (5)	−0.0065 (4)	−0.0009 (4)	−0.0024 (4)
C3	0.0148 (5)	0.0150 (5)	0.0139 (5)	−0.0029 (4)	−0.0017 (4)	−0.0028 (4)
C4	0.0133 (5)	0.0151 (5)	0.0143 (5)	−0.0033 (4)	0.0031 (4)	−0.0027 (4)
C5	0.0114 (5)	0.0169 (5)	0.0181 (5)	−0.0052 (4)	−0.0001 (4)	−0.0016 (4)
C6	0.0141 (5)	0.0194 (5)	0.0144 (5)	−0.0061 (4)	−0.0003 (4)	−0.0031 (4)
C7	0.0210 (6)	0.0246 (6)	0.0170 (5)	−0.0091 (5)	−0.0039 (4)	−0.0045 (4)
C8	0.0253 (6)	0.0266 (6)	0.0151 (5)	−0.0088 (5)	0.0036 (5)	−0.0021 (5)
C9	0.0193 (6)	0.0239 (6)	0.0206 (6)	−0.0111 (5)	−0.0029 (4)	−0.0039 (5)
C10	0.0146 (5)	0.0215 (5)	0.0140 (5)	−0.0062 (4)	−0.0009 (4)	−0.0034 (4)
C11	0.0142 (5)	0.0190 (5)	0.0136 (5)	−0.0047 (4)	−0.0010 (4)	−0.0034 (4)
C12	0.0134 (5)	0.0205 (5)	0.0142 (5)	−0.0067 (4)	−0.0009 (4)	−0.0017 (4)
C13	0.0178 (5)	0.0192 (5)	0.0165 (5)	−0.0080 (4)	−0.0001 (4)	−0.0028 (4)
C14	0.0138 (5)	0.0207 (5)	0.0143 (5)	−0.0072 (4)	0.0025 (4)	−0.0029 (4)
C15	0.0167 (5)	0.0197 (5)	0.0158 (5)	−0.0092 (4)	−0.0021 (4)	−0.0051 (4)
C16	0.0162 (5)	0.0231 (6)	0.0217 (6)	−0.0063 (5)	0.0005 (4)	−0.0049 (5)

Geometric parameters (Å, º)

S1—C11	1.7567 (11)	C5—C6	1.3874 (15)
S1—C13	1.7747 (12)	C6—H6	0.942 (14)
O1—C3	1.3629 (13)	C7—H7A	0.971 (15)

O1—C7	1.4405 (14)	C7—H7B	0.979 (15)
O2—C4	1.3762 (13)	C7—H7C	0.994 (15)
O2—C8	1.4320 (15)	C8—H8A	0.969 (16)
O3—C5	1.3714 (13)	C8—H8B	0.988 (15)
O3—C9	1.4312 (14)	C8—H8C	0.977 (17)
O4—C12	1.2134 (14)	C9—H9A	0.980 (15)
O5—C13	1.2067 (14)	C9—H9B	0.966 (14)
O6—C15	1.2191 (14)	C9—H9C	1.001 (14)
N1—C13	1.3851 (14)	C10—C11	1.3466 (15)
N1—C12	1.3900 (14)	C10—H10	0.948 (14)
N1—C14	1.4529 (14)	C11—C12	1.4845 (15)
C1—C6	1.4009 (14)	C14—C15	1.5231 (16)
C1—C2	1.4012 (15)	C14—H14A	1.016 (15)
C1—C10	1.4590 (15)	C14—H14B	0.947 (14)
C2—C3	1.3901 (15)	C15—C16	1.4941 (16)
C2—H2	0.946 (16)	C16—H16A	0.926 (17)
C3—C4	1.4094 (15)	C16—H16B	0.951 (16)
C4—C5	1.3996 (15)	C16—H16C	0.937 (19)

C11—S1—C13	91.48 (5)	H8A—C8—H8C	111.8 (13)
C3—O1—C7	116.50 (9)	H8B—C8—H8C	112.4 (13)
C4—O2—C8	114.25 (8)	O3—C9—H9A	110.0 (8)
C5—O3—C9	115.87 (9)	O3—C9—H9B	106.0 (8)
C13—N1—C12	116.31 (9)	H9A—C9—H9B	111.2 (12)
C13—N1—C14	120.69 (9)	O3—C9—H9C	110.8 (8)
C12—N1—C14	121.22 (9)	H9A—C9—H9C	110.3 (12)
C6—C1—C2	120.03 (10)	H9B—C9—H9C	108.4 (11)
C6—C1—C10	116.52 (9)	C11—C10—C1	130.61 (10)
C2—C1—C10	123.37 (10)	C11—C10—H10	114.0 (9)
C3—C2—C1	119.64 (10)	C1—C10—H10	115.4 (9)
C3—C2—H2	120.0 (9)	C10—C11—C12	119.86 (10)
C1—C2—H2	120.3 (9)	C10—C11—S1	129.49 (9)
O1—C3—C2	124.35 (10)	C12—C11—S1	110.60 (8)
O1—C3—C4	115.33 (9)	O4—C12—N1	123.07 (10)
C2—C3—C4	120.32 (10)	O4—C12—C11	126.41 (10)
O2—C4—C5	120.89 (10)	N1—C12—C11	110.51 (9)
O2—C4—C3	119.44 (9)	O5—C13—N1	124.82 (11)
C5—C4—C3	119.61 (10)	O5—C13—S1	124.25 (9)
O3—C5—C6	123.72 (10)	N1—C13—S1	110.93 (8)
O3—C5—C4	116.29 (10)	N1—C14—C15	111.00 (9)
C6—C5—C4	119.99 (10)	N1—C14—H14A	110.1 (8)
C5—C6—C1	120.34 (10)	C15—C14—H14A	109.8 (8)
C5—C6—H6	120.6 (9)	N1—C14—H14B	109.6 (9)
C1—C6—H6	119.1 (9)	C15—C14—H14B	108.5 (9)
O1—C7—H7A	105.8 (9)	H14A—C14—H14B	107.8 (12)
O1—C7—H7B	108.4 (9)	O6—C15—C16	123.34 (11)
H7A—C7—H7B	109.4 (12)	O6—C15—C14	120.60 (10)
O1—C7—H7C	109.2 (8)	C16—C15—C14	116.04 (10)

H7A—C7—H7C	111.3 (12)	C15—C16—H16A	107.2 (10)
H7B—C7—H7C	112.5 (12)	C15—C16—H16B	111.7 (10)
O2—C8—H8A	108.7 (9)	H16A—C16—H16B	112.3 (14)
O2—C8—H8B	107.5 (9)	C15—C16—H16C	104.2 (11)
H8A—C8—H8B	106.5 (13)	H16A—C16—H16C	109.2 (15)
O2—C8—H8C	109.8 (10)	H16B—C16—H16C	111.7 (14)
C6—C1—C2—C3	−1.73 (17)	C2—C1—C10—C11	−15.5 (2)
C10—C1—C2—C3	−178.19 (10)	C1—C10—C11—C12	172.00 (11)
C7—O1—C3—C2	−1.74 (15)	C1—C10—C11—S1	−5.3 (2)
C7—O1—C3—C4	177.64 (10)	C13—S1—C11—C10	175.08 (11)
C1—C2—C3—O1	178.73 (10)	C13—S1—C11—C12	−2.42 (8)
C1—C2—C3—C4	−0.62 (17)	C13—N1—C12—O4	−176.61 (11)
C8—O2—C4—C5	82.74 (13)	C14—N1—C12—O4	−11.70 (17)
C8—O2—C4—C3	−100.09 (12)	C13—N1—C12—C11	2.50 (14)
O1—C3—C4—O2	6.01 (15)	C14—N1—C12—C11	167.41 (9)
C2—C3—C4—O2	−174.59 (9)	C10—C11—C12—O4	1.81 (18)
O1—C3—C4—C5	−176.78 (10)	S1—C11—C12—O4	179.59 (10)
C2—C3—C4—C5	2.62 (16)	C10—C11—C12—N1	−177.26 (10)
C9—O3—C5—C6	16.49 (16)	S1—C11—C12—N1	0.52 (12)
C9—O3—C5—C4	−163.65 (10)	C12—N1—C13—O5	176.35 (11)
O2—C4—C5—O3	−4.97 (15)	C14—N1—C13—O5	11.36 (18)
C3—C4—C5—O3	177.86 (10)	C12—N1—C13—S1	−4.36 (13)
O2—C4—C5—C6	174.89 (10)	C14—N1—C13—S1	−169.35 (8)
C3—C4—C5—C6	−2.27 (16)	C11—S1—C13—O5	−176.90 (11)
O3—C5—C6—C1	179.79 (10)	C11—S1—C13—N1	3.80 (9)
C4—C5—C6—C1	−0.06 (17)	C13—N1—C14—C15	85.05 (12)
C2—C1—C6—C5	2.08 (17)	C12—N1—C14—C15	−79.20 (12)
C10—C1—C6—C5	178.78 (10)	N1—C14—C15—O6	−0.64 (14)
C6—C1—C10—C11	167.88 (12)	N1—C14—C15—C16	−179.20 (9)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and S1/N1/C11–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O6^{i}	0.942 (14)	2.398 (14)	3.3108 (14)	163.2 (12)
C7—H7*A*···O5^{ii}	0.971 (15)	2.482 (15)	3.4434 (15)	170.4 (13)
C14—H14*A*···O5^{iii}	1.016 (15)	2.335 (15)	3.2659 (14)	151.8 (11)
C7—H7*C*···*Cg*1^{iv}	0.994 (15)	2.755 (15)	3.5131 (14)	133.3 (11)
C9—H9*C*···*Cg*2^{i}	1.001 (14)	2.900 (15)	3.8441 (14)	157.5 (11)

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