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(5E)-5-(4-Hydroxy-3-methoxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one methanol monosolvate

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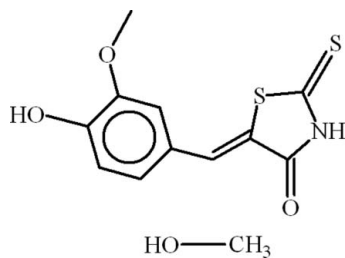
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in solvent or counterion; R factor = 0.039; wR factor = 0.070; data-to-parameter ratio = 13.4.

In the title compound, $\text{C}_{11}\text{H}_9\text{NO}_3\text{S}_2 \cdot \text{CH}_4\text{O}$, the dihedral angle between the aromatic rings is 3.57 (16°) and intramolecular $\text{O}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{S}$ interactions occur. In the crystal, the thiazolidin-4-one molecules are linked by $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds, forming chains. The hydrogen-bond motifs lead to $S(5)$, $S(6)$ and $R_3^2(8)$ ring motifs. There exist $\text{C}=\text{O} \cdots \pi$ interactions between the heterocyclic rings and $\pi-\pi$ interactions between the heterocyclic and benzene rings at distances of 3.455 (2) and 3.602 (2) Å, respectively. The methanol solvent molecule is disordered over two sets of sites in a 0.542 (9): 0.458 (9) ratio.

Related literature

For related structures, see: Barreiro *et al.* (2007); Shahwar *et al.* (2009). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{11}\text{H}_9\text{NO}_3\text{S}_2 \cdot \text{CH}_4\text{O}$
 $M_r = 299.35$
 Orthorhombic, $Pna2_1$
 $a = 17.731$ (2) Å

$b = 11.7528$ (14) Å
 $c = 6.5715$ (6) Å
 $V = 1369.4$ (3) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.40$ mm⁻¹

$T = 296$ K
 $0.26 \times 0.13 \times 0.12$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.942$, $T_{\max} = 0.955$

7574 measured reflections
 2472 independent reflections
 1807 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.070$
 $S = 1.02$
 2472 reflections
 185 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³
 Absolute structure: Flack (1983), 829 Friedel Pairs
 Flack parameter: 0.01 (8)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}-\text{H1} \cdots \text{O2}$	0.88 (3)	2.21 (3)	2.641 (3)	109 (3)
$\text{C2}-\text{H2} \cdots \text{S1}$	0.93	2.66	3.349 (3)	132
$\text{O1}-\text{H1} \cdots \text{O4A}^i$	0.88 (3)	1.85 (3)	2.622 (7)	145 (3)
$\text{N1}-\text{H1N} \cdots \text{O1}^{ii}$	0.86	2.05	2.899 (3)	169
$\text{O4A}-\text{H4A} \cdots \text{O3}^{iii}$	0.96 (8)	1.79 (8)	2.744 (7)	173 (7)
$\text{C12A}-\text{H12A} \cdots \text{O3}^{iv}$	0.96	2.37	3.150 (5)	139

Symmetry codes: (i) $x, y, z + 1$; (ii) $-x + \frac{1}{2}, y - \frac{1}{2}, z - \frac{3}{2}$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, z$. Cg2 is the centroid of the C1-C6 benzene ring.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and PLATON (Spek, 2009); 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: HB5118).

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supporting information

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(5*E*)-5-(4-Hydroxy-3-methoxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one methanol monosolvate

Durre Shahwar, M. Nawaz Tahir, Muhammad Asam Raza, Maria Saddaf and Sana Majeed

S1. Comment

We have recently reported the crystal structure of (5*Z*)-5-(2-Hydroxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one - methanol (1:0.5) (Shahwar *et al.*, 2009). In continuation of synthesizing various derivatives of rhodanine, the title compound (I, Fig. 1), is being reported.

The crystal structure of (II) 5-(4-Hydroxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one dimethylsulfoxide solvate (Barreiro, *et al.*, 2007) has been published. The title compound (I) differs from (II) due to attachment of methoxy group adjacent to the hydroxy group and due to solvate i.e methanol instead of dimethylsulfoxide.

In the title molecule there exist intermolecular H-bondings of O—H \cdots O, C—H \cdots O and S—H \cdots O types (Table 1, Fig. 1) forming two S(5) and one S(6) ring motif (Bernstein *et al.*, 1995). The role of disordered methanol solvate is to interlink the molecules through O—H \cdots O type of H-bondings forming $R_3^3(8)$ ring motifs (Fig. 2). The molecules are stabilized in the form of infinite one dimensional polymeric chains. There exist π - π interactions between the centroids of heterocyclic ring *Cg*1 (C8/C9/N1/C10/S1) and the benzene ring *Cg*2 (C1—C6). The distance between the centroids *Cg*1 \rightarrow *Cg*2 is 3.455 (2) Å due to symmetry ($x, y, \mp 1 + z$) and for *Cg*2 \rightarrow *Cg*1 is 3.602 (2) Å due to symmetry ($1/2 - x, \mp 1/2 + y, \mp 1/2 + z$), respectively. The molecules may also be stabilized due C=O \cdots π interaction (Table 1). The methanol molecule is disordered over two sites with an occupancy ratio of 0.542 (9):0.458 (9).

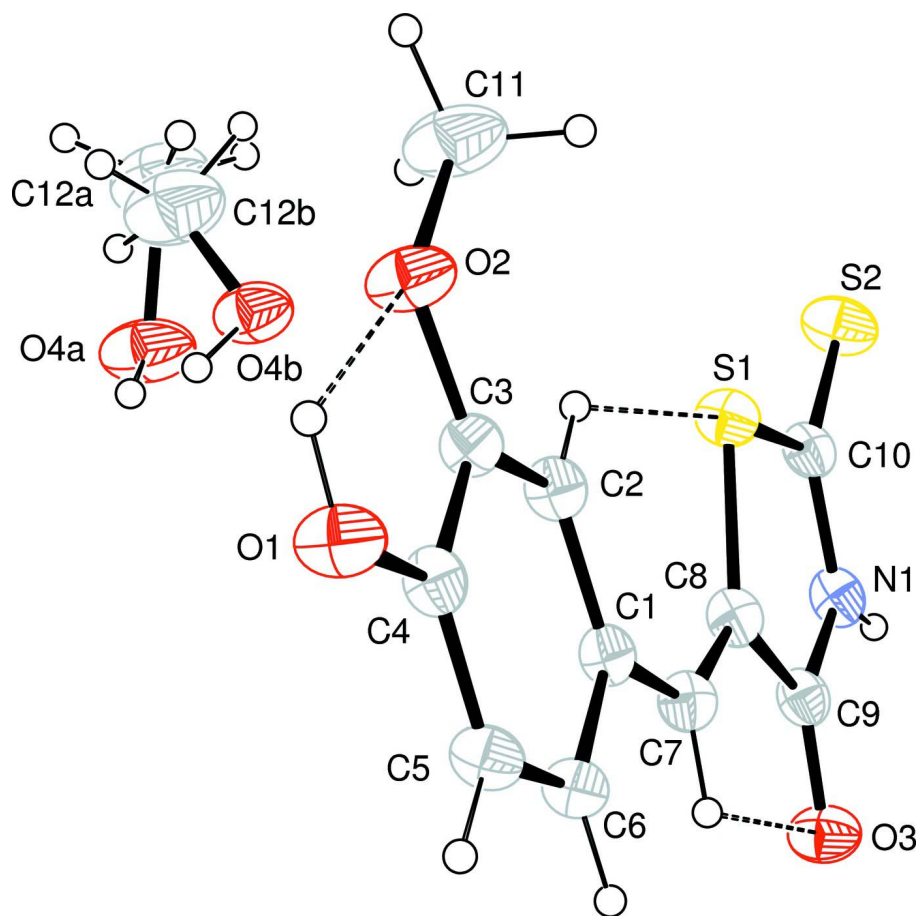
S2. Experimental

Rhodanine (0.266 g, 0.2 mol), 4-hydroxy-3-methoxybenzaldehyde (0.304 g, 0.2 mol) and K₂CO₃ (0.553 g, 0.4 mol) were dissolved in 10 ml distilled water at room temperature. The stirring was continued for 24 h and reaction was monitored by TLC. The precipitates were formed during neutralization of the reaction mixture with 5% HCl. The precipitates were filtered off and washed with saturated solution of NaCl. The crude material obtained was recrystallized in methanol to afford dark brown needles of (I).

S3. Refinement

The coordinates of H1 and H4A attached with O1 and O4A respectively, were refined.

The H-atoms were positioned geometrically with O—H = 0.82, N—H = 0.86, C—H = 0.93 and 0.96 Å for aromatic like and methyl H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C, N, O})$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms.

**Figure 1**

View of (I) with displacement ellipsoids drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radius. The dotted line represent the intramolecular H-bond.

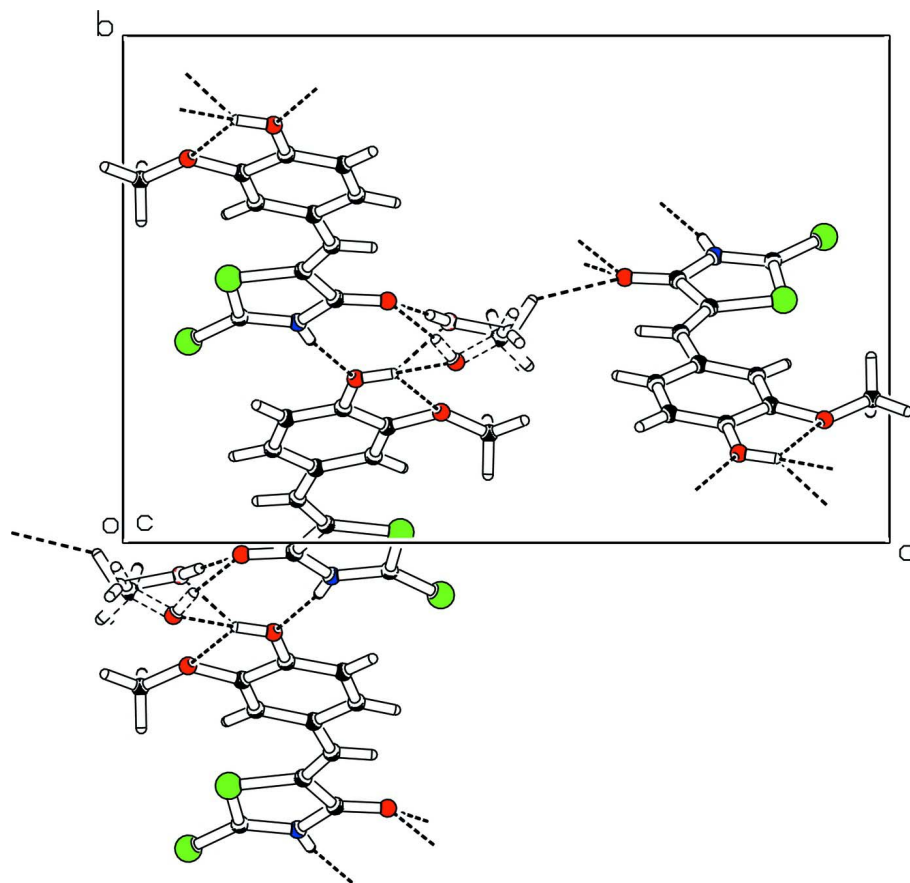


Figure 2

The partial packing of (I), which shows that molecules form polymeric chains.

(5*E*)-5-(4-Hydroxy-3-methoxybenzylidene)-2-thioxo-1,3-thiazolidin-4-one methanol monosolvate

Crystal data

$C_{11}H_9NO_3S_2 \cdot CH_4O$

$M_r = 299.35$

Orthorhombic, $Pna2_1$

Hall symbol: $P\ 2c\ -2n$

$a = 17.731\ (2)\ \text{\AA}$

$b = 11.7528\ (14)\ \text{\AA}$

$c = 6.5715\ (6)\ \text{\AA}$

$V = 1369.4\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 624$

$D_x = 1.452\ \text{Mg m}^{-3}$

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

Cell parameters from 2472 reflections

$\theta = 2.9\text{--}27.1^\circ$

$\mu = 0.40\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Cut needle, dark brown

$0.26 \times 0.13 \times 0.12\ \text{mm}$

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $7.50\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2007)

$T_{\min} = 0.942$, $T_{\max} = 0.955$

7574 measured reflections

2472 independent reflections

1807 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 27.1^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -22 \rightarrow 22$

$k = -13 \rightarrow 15$

$l = -5 \rightarrow 8$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.070$ $S = 1.02$

2472 reflections

185 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0145P)^2 + 0.2762P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$ Absolute structure: Flack (1983), 829 Friedal
Pairs

Absolute structure parameter: 0.01 (8)

*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 (\AA^2)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.36194 (4)	0.02090 (7)	0.57918 (14)	0.0440 (3)	
S2	0.41466 (5)	-0.10304 (9)	0.20833 (15)	0.0609 (4)	
O1	0.30380 (12)	0.3234 (2)	1.4811 (3)	0.0514 (9)	
O2	0.41511 (11)	0.2575 (2)	1.2416 (3)	0.0540 (9)	
O3	0.15476 (12)	-0.0232 (2)	0.4387 (3)	0.0531 (9)	
N1	0.27209 (14)	-0.0654 (2)	0.3174 (4)	0.0403 (9)	
C1	0.25139 (18)	0.1479 (3)	0.9536 (4)	0.0352 (10)	
C2	0.32661 (18)	0.1714 (3)	1.0013 (5)	0.0383 (11)	
C3	0.34462 (16)	0.2296 (3)	1.1767 (5)	0.0377 (11)	
C4	0.28684 (17)	0.2662 (3)	1.3082 (4)	0.0373 (11)	
C5	0.21274 (17)	0.2455 (3)	1.2609 (5)	0.0412 (11)	
C6	0.19503 (16)	0.1858 (3)	1.0864 (5)	0.0411 (11)	
C7	0.22722 (18)	0.0873 (3)	0.7745 (5)	0.0410 (11)	
C8	0.26494 (16)	0.0363 (3)	0.6206 (4)	0.0376 (11)	
C9	0.22317 (17)	-0.0188 (3)	0.4558 (5)	0.0405 (11)	
C10	0.34766 (17)	-0.0547 (3)	0.3526 (5)	0.0392 (11)	
C11	0.47733 (18)	0.2154 (4)	1.1321 (6)	0.0780 (18)	
O4A	0.4252 (3)	0.4356 (7)	0.5888 (10)	0.078 (3)	0.542 (9)
C12A	0.5055 (2)	0.4123 (5)	0.6066 (13)	0.096 (2)	0.542 (9)
O4B	0.4343 (2)	0.3568 (4)	0.6677 (9)	0.059 (3)	0.458 (9)
C12B	0.4913 (2)	0.4044 (4)	0.6141 (9)	0.096 (2)	0.458 (9)
H1	0.3525 (17)	0.334 (3)	1.499 (5)	0.0617*	
H1N	0.25564	-0.10029	0.21132	0.0483*	
H2	0.36478	0.14769	0.91393	0.0460*	

H5	0.17457	0.27152	1.34604	0.0495*	
H6	0.14477	0.17047	1.05653	0.0492*	
H7	0.17507	0.08219	0.76231	0.0494*	
H11A	0.47613	0.13375	1.13217	0.1166*	
H11B	0.52316	0.24114	1.19480	0.1166*	
H11C	0.47516	0.24266	0.99447	0.1166*	
H4A	0.401 (4)	0.449 (6)	0.717 (13)	0.0935*	0.542 (9)
H12C	0.51734	0.39385	0.74524	0.1441*	0.542 (9)
H12A	0.53358	0.47831	0.56588	0.1441*	0.542 (9)
H12B	0.51849	0.34937	0.52036	0.1441*	0.542 (9)
H4B	0.40848	0.40061	0.73547	0.0709*	0.458 (9)
H12D	0.50918	0.45230	0.72210	0.1441*	0.458 (9)
H12E	0.48086	0.44993	0.49615	0.1441*	0.458 (9)
H12F	0.52902	0.34877	0.58154	0.1441*	0.458 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0445 (4)	0.0523 (5)	0.0353 (4)	0.0038 (4)	-0.0056 (4)	-0.0094 (5)
S2	0.0552 (5)	0.0804 (8)	0.0472 (5)	0.0164 (5)	0.0008 (5)	-0.0137 (6)
O1	0.0444 (14)	0.0726 (19)	0.0372 (13)	0.0026 (13)	0.0019 (11)	-0.0231 (12)
O2	0.0383 (13)	0.0796 (17)	0.0442 (14)	-0.0046 (12)	0.0060 (11)	-0.0230 (13)
O3	0.0435 (13)	0.0691 (18)	0.0467 (14)	0.0004 (12)	-0.0084 (11)	-0.0146 (13)
N1	0.0527 (17)	0.0388 (18)	0.0293 (14)	0.0048 (14)	-0.0049 (12)	-0.0101 (13)
C1	0.0417 (17)	0.0343 (19)	0.0295 (17)	0.0022 (14)	0.0031 (14)	-0.0013 (14)
C2	0.0442 (19)	0.041 (2)	0.0297 (17)	0.0029 (16)	0.0060 (14)	-0.0062 (16)
C3	0.0389 (17)	0.040 (2)	0.0341 (19)	0.0002 (15)	0.0035 (15)	-0.0030 (17)
C4	0.047 (2)	0.037 (2)	0.0278 (18)	0.0023 (15)	0.0007 (15)	-0.0093 (16)
C5	0.0414 (19)	0.051 (2)	0.0313 (18)	0.0070 (17)	0.0024 (15)	-0.0069 (16)
C6	0.0372 (17)	0.045 (2)	0.0410 (18)	0.0037 (14)	-0.0008 (18)	-0.001 (2)
C7	0.0437 (18)	0.041 (2)	0.0383 (19)	0.0002 (16)	-0.0016 (15)	0.0005 (17)
C8	0.0464 (17)	0.039 (2)	0.0275 (19)	0.0024 (14)	-0.0081 (14)	-0.0034 (15)
C9	0.048 (2)	0.037 (2)	0.0364 (18)	0.0040 (17)	-0.0041 (16)	-0.0005 (16)
C10	0.047 (2)	0.038 (2)	0.0327 (18)	0.0049 (15)	-0.0088 (15)	-0.0018 (15)
C11	0.044 (2)	0.113 (4)	0.077 (3)	-0.005 (2)	0.0177 (18)	-0.026 (3)
O4A	0.048 (3)	0.119 (6)	0.067 (4)	0.004 (3)	0.005 (3)	-0.039 (5)
C12A	0.064 (3)	0.131 (5)	0.093 (4)	-0.008 (3)	0.011 (3)	-0.019 (4)
O4B	0.043 (3)	0.079 (6)	0.055 (4)	-0.001 (3)	0.006 (3)	-0.020 (4)
C12B	0.064 (3)	0.131 (5)	0.093 (4)	-0.008 (3)	0.011 (3)	-0.019 (4)

Geometric parameters (Å, °)

S1—C8	1.751 (3)	C3—C4	1.408 (4)
S1—C10	1.752 (3)	C4—C5	1.372 (4)
S2—C10	1.623 (3)	C5—C6	1.381 (5)
O1—C4	1.354 (4)	C7—C8	1.353 (4)
O2—C3	1.361 (4)	C8—C9	1.463 (4)
O2—C11	1.407 (4)	C2—H2	0.9300

O3—C9	1.219 (4)	C5—H5	0.9300
O1—H1	0.88 (3)	C6—H6	0.9300
O4A—C12A	1.455 (7)	C7—H7	0.9300
O4B—C12B	1.208 (6)	C11—H11A	0.9600
O4A—H4A	0.96 (8)	C11—H11B	0.9600
O4B—H4B	0.8200	C11—H11C	0.9600
N1—C10	1.366 (4)	C12A—H12B	0.9600
N1—C9	1.371 (4)	C12A—H12C	0.9600
N1—H1N	0.8600	C12A—H12A	0.9600
C1—C2	1.398 (5)	C12B—H12D	0.9600
C1—C7	1.441 (4)	C12B—H12E	0.9600
C1—C6	1.400 (4)	C12B—H12F	0.9600
C2—C3	1.378 (5)		
C8—S1—C10	92.44 (14)	S2—C10—N1	126.0 (3)
C3—O2—C11	118.4 (3)	S1—C10—S2	124.63 (19)
C4—O1—H1	114 (2)	C3—C2—H2	120.00
C12A—O4A—H4A	114 (4)	C1—C2—H2	120.00
C12B—O4B—H4B	110.00	C4—C5—H5	120.00
C9—N1—C10	118.1 (3)	C6—C5—H5	120.00
C10—N1—H1N	121.00	C5—C6—H6	119.00
C9—N1—H1N	121.00	C1—C6—H6	119.00
C2—C1—C7	124.4 (3)	C8—C7—H7	113.00
C2—C1—C6	118.6 (3)	C1—C7—H7	113.00
C6—C1—C7	117.0 (3)	O2—C11—H11C	109.00
C1—C2—C3	120.5 (3)	O2—C11—H11A	110.00
O2—C3—C4	113.7 (3)	O2—C11—H11B	109.00
O2—C3—C2	126.5 (3)	H11B—C11—H11C	109.00
C2—C3—C4	119.8 (3)	H11A—C11—H11B	109.00
O1—C4—C5	119.4 (3)	H11A—C11—H11C	109.00
C3—C4—C5	120.3 (3)	O4A—C12A—H12B	109.00
O1—C4—C3	120.4 (3)	O4A—C12A—H12C	109.00
C4—C5—C6	119.8 (3)	O4A—C12A—H12A	109.00
C1—C6—C5	121.2 (3)	H12A—C12A—H12C	109.00
C1—C7—C8	133.1 (3)	H12B—C12A—H12C	110.00
S1—C8—C9	109.7 (2)	H12A—C12A—H12B	109.00
S1—C8—C7	130.4 (2)	O4B—C12B—H12D	109.00
C7—C8—C9	120.0 (3)	O4B—C12B—H12E	109.00
O3—C9—C8	126.2 (3)	O4B—C12B—H12F	109.00
N1—C9—C8	110.3 (3)	H12D—C12B—H12E	110.00
O3—C9—N1	123.5 (3)	H12D—C12B—H12F	110.00
S1—C10—N1	109.4 (2)	H12E—C12B—H12F	110.00
C10—S1—C8—C7	179.4 (4)	C1—C2—C3—O2	179.7 (3)
C10—S1—C8—C9	0.3 (3)	C1—C2—C3—C4	-0.4 (5)
C8—S1—C10—S2	179.6 (3)	O2—C3—C4—O1	-0.1 (5)
C8—S1—C10—N1	-0.1 (3)	O2—C3—C4—C5	179.1 (3)
C11—O2—C3—C2	-6.2 (5)	C2—C3—C4—O1	180.0 (3)

C11—O2—C3—C4	173.9 (3)	C2—C3—C4—C5	-0.9 (5)
C10—N1—C9—O3	179.8 (3)	O1—C4—C5—C6	-179.1 (3)
C10—N1—C9—C8	0.4 (4)	C3—C4—C5—C6	1.8 (5)
C9—N1—C10—S1	-0.2 (4)	C4—C5—C6—C1	-1.4 (5)
C9—N1—C10—S2	-179.8 (3)	C1—C7—C8—S1	1.4 (6)
C6—C1—C2—C3	0.7 (5)	C1—C7—C8—C9	-179.5 (4)
C7—C1—C2—C3	-179.7 (3)	S1—C8—C9—O3	-179.8 (3)
C2—C1—C6—C5	0.2 (5)	S1—C8—C9—N1	-0.4 (3)
C7—C1—C6—C5	-179.4 (3)	C7—C8—C9—O3	1.0 (5)
C2—C1—C7—C8	3.1 (6)	C7—C8—C9—N1	-179.6 (3)
C6—C1—C7—C8	-177.4 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots O2	0.88 (3)	2.21 (3)	2.641 (3)	109 (3)
C2—H2 \cdots S1	0.93	2.66	3.349 (3)	132
O1—H1 \cdots O4A ⁱ	0.88 (3)	1.85 (3)	2.622 (7)	145 (3)
N1—H1N \cdots O1 ⁱⁱ	0.86	2.05	2.899 (3)	169
O4A—H4A \cdots O3 ⁱⁱⁱ	0.96 (8)	1.79 (8)	2.744 (7)	173 (7)
C12A—H12A \cdots O3 ^{iv}	0.96	2.37	3.150 (5)	139

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+1/2, y-1/2, z-3/2$; (iii) $-x+1/2, y+1/2, z+1/2$; (iv) $x+1/2, -y+1/2, z$.