

## 5-[[2-Hydroxyethyl)sulfanyl]methyl]quinolin-8-ol

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Received 29 April 2019

Accepted 3 May 2019

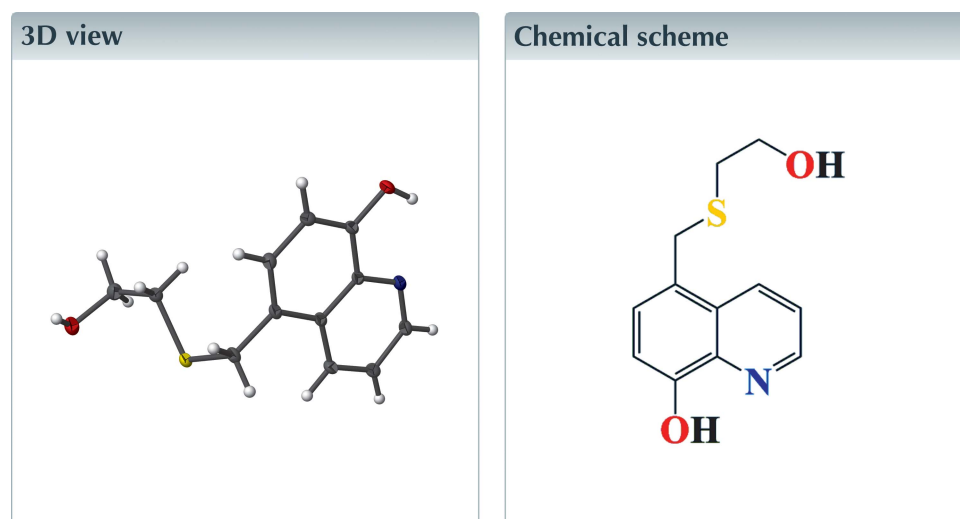
Edited by L. Van Meervelt, Katholieke Universiteit Leuven, Belgium

Keywords: crystal structure; hydrogen bond;  $\pi$ -stacking; quinolinol.

CCDC reference: 1913753

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

In the title molecule,  $C_{12}H_{13}NO_2S$ , the quinolinol unit is planar (r.m.s. deviation = 0.0128 Å). In the crystal,  $O-H\cdots N$  and  $O-H\cdots S$  hydrogen bonds together with  $\pi$ -stacking interactions form layers parallel to [100] that are associated through  $C-H\cdots O$  hydrogen bonds.

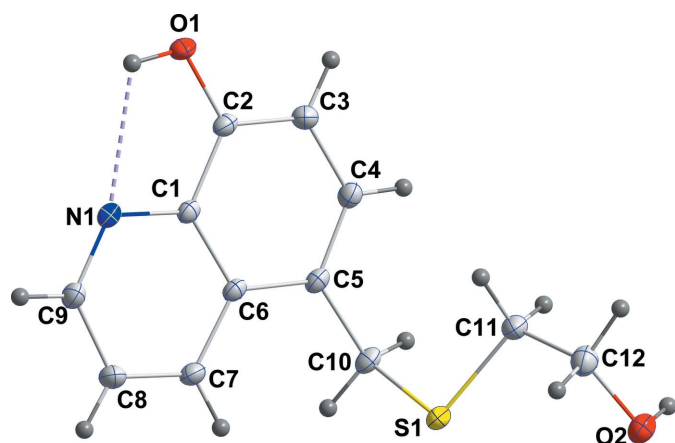


## Structure description

Organic synthesis is a major tool for the formation of new biologically active molecules, in particular heterocyclic molecules (Rbaa *et al.*, 2018). 8-Hydroxyquinoline is an important heterocyclic nucleus, thanks to its structure which presents various nucleophilic and electrophilic reactive sites that allow the synthesis of new heterocyclic derivatives. Following our interest in 8-quinolinol-based biological and anti-corrosion inhibitor compounds (El Faydy *et al.*, 2016; Rbaa *et al.* 2017), we have synthesized the title compound by reaction of 5-chloromethylquinoline-8-ol hydrochloride with thioethanol in the presence of triethylamine in pure tetrahydrofuran as a solvent.

The quinolinol unit is planar to within 0.0200 (9) Å (r.m.s. deviation of the fitted atoms = 0.0128 Å) with C8 farthest from the mean plane. The side chain attached to C5 is nearly perpendicular to this plane as indicated by the C4–C5–C10–S1 torsion angle of 99.16 (10)°. There is a hydrogen bond between the oxygen atom of the phenolic ring O1 and the nitrogen atom of the pyridine ring N1 (Fig. 1, Table 1).

In the crystal, the molecules form inversion dimers through  $O1-H1\cdots N1^i$  hydrogen bonds with a  $R_2^2(10)$  graph set (Table 1 and Fig. 2). These are connected into layers parallel to [100] by  $O2-H2\cdots S1^{ii}$  hydrogen bonds and  $\pi$ -stacking interactions between inversion-related C1–C6 rings [centroid–centroid distance = 3.4044 (6) Å]. In the layers, the hydroxyethyl groups extend on either side, engaging in  $C7-H7\cdots O2^{ii}$  and  $C8-$

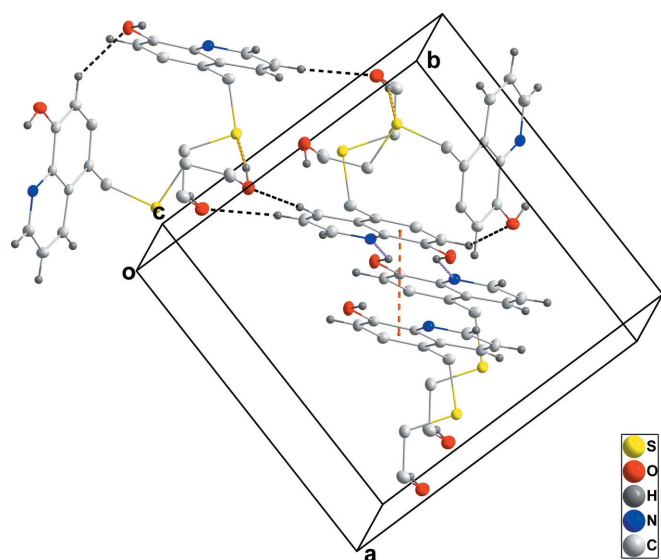


**Figure 1**  
The title molecule with the atom-labelling scheme and 50% probability ellipsoids. The intramolecular O—H···N hydrogen bond is shown by a dashed line.

H8···O2<sup>iii</sup> hydrogen bonds, which tie the layers together (Table 1 and Figs. 2–4). C9—H9···O1<sup>i</sup> hydrogen bonds also occur.

### Synthesis and crystallization

A mixture of 5-chloromethyl-8-hydroxyquinoline hydrochloride (0.01 mol), and thioethanol (0.02 mol) in 50 ml of absolute tetrahydrofuran (THF) in the presence of NaHCO<sub>3</sub> was refluxed under magnetic stirring for 8 h. The reaction was followed by TLC, after cooling. The reaction mixture was then added to 20 ml of water and then extracted with dichloromethane (3 × 20 ml). The organic layers were combined, washed twice with saturated aqueous sodium chloride, dried over anhydrous magnesium sulfate and concentrated to

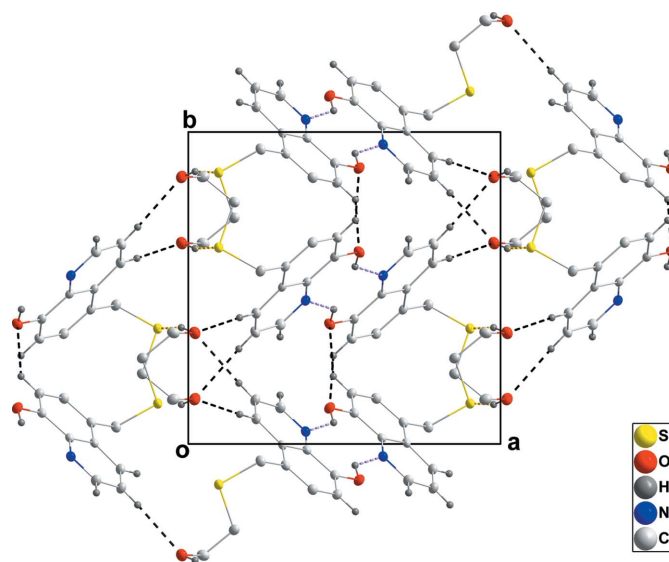


**Figure 2**  
Detail of the intermolecular interactions. O—H···N, C—H···O and C—H···S hydrogen bonds are shown, respectively, by light-purple, black and gold dashed lines. The  $\pi$ -stacking interaction is shown by an orange dashed line.

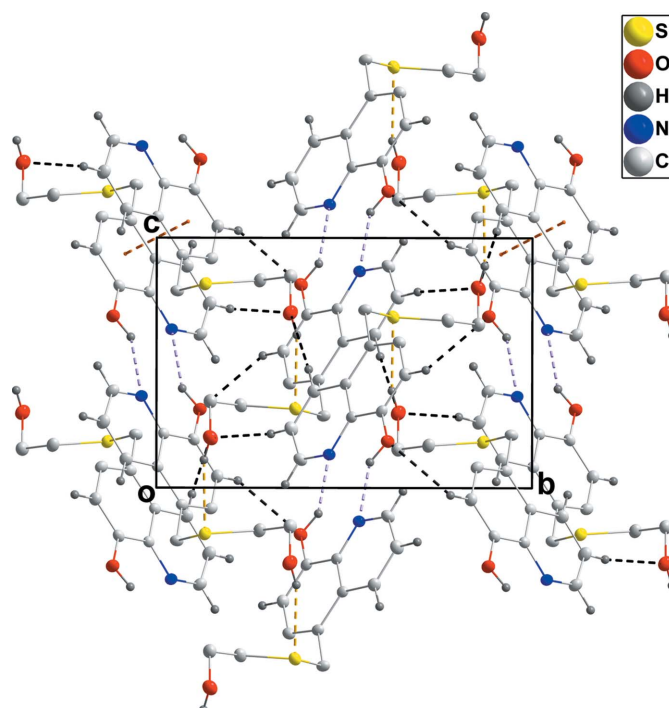
**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···N1	0.87	2.29	2.7577 (12)	114
O1—H1···N1 <sup>i</sup>	0.87	2.19	2.8395 (11)	131
O2—H2···S1 <sup>ii</sup>	0.87	2.47	3.2919 (9)	159
C3—H3···O1 <sup>iii</sup>	0.955 (16)	2.599 (16)	3.2858 (13)	129.1 (11)
C8—H8···O2 <sup>iii</sup>	0.903 (17)	2.529 (17)	3.4252 (14)	171.9 (14)
C9—H9···O1 <sup>i</sup>	0.917 (16)	2.525 (16)	3.0446 (13)	116.3 (12)

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



**Figure 3**  
Packing viewed along the *c*-axis direction with intermolecular interactions depicted as in Fig. 2.



**Figure 4**  
Packing viewed along the *a*-axis direction with intermolecular interactions depicted as in Fig. 2.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>12</sub> H <sub>13</sub> NO <sub>2</sub> S
<i>M<sub>r</sub></i>	235.29
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	120
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.8362 (7), 11.7958 (7), 7.8459 (5)
$\beta$ (°)	91.673 (1)
<i>V</i> (Å <sup>3</sup> )	1094.96 (12)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.28
Crystal size (mm)	0.44 × 0.43 × 0.23
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> – <i>T</i> <sub>max</sub>	0.86, 0.94
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	33009, 2961, 2797
<i>R</i> <sub>int</sub>	0.025
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.687
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.032, 0.093, 1.05
No. of reflections	2961
No. of parameters	191
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.56, -0.20

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/1* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

dryness on a rotary evaporator. The product was then purified by silica column chromatography using a mixture of acetone/

hexane (85:15, *v/v*), and recrystallized from ethanol solution to give crystals suitable for X-ray analysis.

## Refinement

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

## Acknowledgements

We thank Ibn Tofail University and Mohammed V University for supporting this study and Tulane University for support of the Tulane Crystallography Laboratory.

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## full crystallographic data

*IUCrData* (2019). 4, x190625 [https://doi.org/10.1107/S2414314619006254]

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## 5-[[2-Hydroxyethyl)sulfanyl]methyl]quinolin-8-ol

*Crystal data*

$C_{12}H_{13}NO_2S$

$M_r = 235.29$

Monoclinic,  $P2_1/c$

$a = 11.8362$  (7) Å

$b = 11.7958$  (7) Å

$c = 7.8459$  (5) Å

$\beta = 91.673$  (1)°

$V = 1094.96$  (12) Å<sup>3</sup>

$Z = 4$

$F(000) = 496$

$D_x = 1.427$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 9809 reflections

$\theta = 2.4$ – $29.2$ °

$\mu = 0.28$  mm<sup>-1</sup>

$T = 120$  K

Thick plate, colourless

$0.44 \times 0.43 \times 0.23$  mm

*Data collection*

Bruker SMART APEX CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3333 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.86$ ,  $T_{\max} = 0.94$

33009 measured reflections

2961 independent reflections

2797 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 29.2$ °,  $\theta_{\min} = 1.7$ °

$h = -16 \rightarrow 16$

$k = -15 \rightarrow 16$

$l = -10 \rightarrow 10$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.093$

$S = 1.05$

2961 reflections

191 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.4352P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.56$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

*Special details*

**Experimental.** The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in  $\omega$ , collected at  $\varphi = 0.00$ , 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in  $\varphi$ , collected at  $\omega = -30.00$  and 210.00°. The scan time was 5 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  $F^2 > 2\sigma(F^2)$  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. The hydrogen atoms attached to oxygen were placed in locations derived from a difference map, their coordinates adjusted to give O—H = 0.87 %Å and were included as riding contributions.

The hydrogen atoms attached to oxygen were placed in locations derived from a difference map, their coordinates adjusted to give O—H = 0.87 Å and were included as riding contributions.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.09756 (2)	0.62998 (2)	0.68410 (3)	0.01569 (9)
O1	0.54726 (7)	0.61574 (7)	0.18639 (10)	0.01798 (17)
H1	0.534302	0.568575	0.102876	0.039 (5)*
O2	−0.02097 (7)	0.85612 (7)	0.79986 (11)	0.02225 (18)
H2	0.021957	0.873272	0.888036	0.065 (7)*
N1	0.37596 (7)	0.46007 (7)	0.13362 (11)	0.01481 (18)
C1	0.37994 (8)	0.51945 (8)	0.28340 (12)	0.01271 (19)
C2	0.46902 (8)	0.59965 (9)	0.30686 (13)	0.01415 (19)
C3	0.47685 (9)	0.66206 (9)	0.45413 (13)	0.0163 (2)
H3	0.5355 (13)	0.7169 (13)	0.4712 (19)	0.022 (4)*
C4	0.39811 (9)	0.64610 (9)	0.58290 (13)	0.0157 (2)
H4	0.4071 (13)	0.6887 (13)	0.683 (2)	0.021 (3)*
C5	0.31138 (8)	0.56882 (9)	0.56841 (12)	0.01389 (19)
C6	0.30114 (8)	0.50343 (8)	0.41551 (12)	0.01284 (19)
C7	0.21737 (8)	0.41920 (9)	0.38675 (13)	0.0163 (2)
H7	0.1644 (13)	0.4049 (13)	0.474 (2)	0.021 (4)*
C8	0.21448 (9)	0.35904 (9)	0.23679 (14)	0.0183 (2)
H8	0.1620 (14)	0.3049 (14)	0.216 (2)	0.026 (4)*
C9	0.29511 (9)	0.38318 (9)	0.11339 (14)	0.0173 (2)
H9	0.2941 (13)	0.3434 (13)	0.013 (2)	0.022 (4)*
C10	0.23173 (9)	0.55471 (9)	0.71246 (13)	0.0157 (2)
H10A	0.2690 (13)	0.5808 (13)	0.817 (2)	0.021 (3)*
H10B	0.2087 (13)	0.4760 (14)	0.7278 (19)	0.023 (4)*
C11	0.14715 (9)	0.77525 (9)	0.66999 (14)	0.0182 (2)
H11A	0.1931 (13)	0.7926 (14)	0.771 (2)	0.025 (4)*
H11B	0.1940 (14)	0.7851 (15)	0.568 (2)	0.030 (4)*
C12	0.04781 (10)	0.85674 (10)	0.65398 (15)	0.0210 (2)
H12A	0.0778 (13)	0.9341 (14)	0.633 (2)	0.027 (4)*
H12B	−0.0047 (14)	0.8363 (14)	0.560 (2)	0.025 (4)*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.01307 (14)	0.01642 (14)	0.01784 (14)	0.00009 (8)	0.00495 (9)	−0.00174 (8)

O1	0.0179 (4)	0.0194 (4)	0.0170 (4)	-0.0042 (3)	0.0076 (3)	-0.0010 (3)
O2	0.0195 (4)	0.0236 (4)	0.0240 (4)	0.0021 (3)	0.0054 (3)	-0.0036 (3)
N1	0.0140 (4)	0.0165 (4)	0.0141 (4)	0.0013 (3)	0.0028 (3)	-0.0006 (3)
C1	0.0118 (4)	0.0129 (4)	0.0135 (4)	0.0023 (3)	0.0021 (3)	0.0009 (3)
C2	0.0128 (4)	0.0143 (4)	0.0155 (4)	0.0014 (3)	0.0038 (3)	0.0025 (3)
C3	0.0145 (4)	0.0160 (4)	0.0184 (5)	-0.0019 (4)	0.0024 (4)	-0.0006 (4)
C4	0.0152 (5)	0.0174 (5)	0.0146 (4)	0.0014 (4)	0.0015 (4)	-0.0017 (3)
C5	0.0126 (4)	0.0159 (4)	0.0132 (4)	0.0031 (3)	0.0027 (3)	0.0008 (3)
C6	0.0109 (4)	0.0140 (4)	0.0137 (4)	0.0025 (3)	0.0023 (3)	0.0012 (3)
C7	0.0130 (4)	0.0178 (5)	0.0185 (5)	-0.0003 (4)	0.0047 (4)	0.0002 (4)
C8	0.0143 (5)	0.0193 (5)	0.0215 (5)	-0.0031 (4)	0.0036 (4)	-0.0030 (4)
C9	0.0161 (5)	0.0192 (5)	0.0167 (5)	-0.0003 (4)	0.0035 (4)	-0.0037 (4)
C10	0.0152 (4)	0.0192 (5)	0.0129 (4)	0.0022 (4)	0.0037 (3)	0.0011 (3)
C11	0.0175 (5)	0.0169 (5)	0.0205 (5)	-0.0015 (4)	0.0061 (4)	-0.0018 (4)
C12	0.0239 (5)	0.0186 (5)	0.0206 (5)	0.0025 (4)	0.0042 (4)	0.0001 (4)

*Geometric parameters (Å, °)*

S1—C11	1.8158 (11)	C5—C6	1.4284 (13)
S1—C10	1.8273 (11)	C5—C10	1.5021 (13)
O1—C2	1.3558 (12)	C6—C7	1.4171 (14)
O1—H1	0.8698	C7—C8	1.3736 (15)
O2—C12	1.4239 (14)	C7—H7	0.956 (16)
O2—H2	0.8701	C8—C9	1.4082 (15)
N1—C9	1.3246 (14)	C8—H8	0.903 (17)
N1—C1	1.3677 (13)	C9—H9	0.916 (16)
C1—C2	1.4245 (14)	C10—H10A	0.969 (15)
C1—C6	1.4271 (13)	C10—H10B	0.976 (16)
C2—C3	1.3709 (14)	C11—C12	1.5211 (16)
C3—C4	1.4070 (14)	C11—H11A	0.967 (16)
C3—H3	0.955 (16)	C11—H11B	0.993 (17)
C4—C5	1.3751 (14)	C12—H12A	0.994 (17)
C4—H4	0.934 (16)	C12—H12B	0.978 (16)
C11—S1—C10	100.64 (5)	C7—C8—C9	118.95 (10)
C2—O1—H1	109.1	C7—C8—H8	121.5 (10)
C12—O2—H2	107.7	C9—C8—H8	119.6 (10)
C9—N1—C1	117.41 (9)	N1—C9—C8	123.90 (10)
N1—C1—C2	117.26 (9)	N1—C9—H9	116.4 (10)
N1—C1—C6	123.32 (9)	C8—C9—H9	119.7 (10)
C2—C1—C6	119.41 (9)	C5—C10—S1	114.64 (7)
O1—C2—C3	118.79 (9)	C5—C10—H10A	108.7 (9)
O1—C2—C1	121.39 (9)	S1—C10—H10A	108.7 (9)
C3—C2—C1	119.81 (9)	C5—C10—H10B	112.5 (9)
C2—C3—C4	120.23 (10)	S1—C10—H10B	103.4 (9)
C2—C3—H3	120.8 (9)	H10A—C10—H10B	108.7 (12)
C4—C3—H3	118.9 (9)	C12—C11—S1	110.55 (8)
C5—C4—C3	122.54 (9)	C12—C11—H11A	110.4 (9)

C5—C4—H4	119.4 (9)	S1—C11—H11A	109.0 (9)
C3—C4—H4	118.0 (9)	C12—C11—H11B	108.0 (10)
C4—C5—C6	118.18 (9)	S1—C11—H11B	110.4 (10)
C4—C5—C10	119.65 (9)	H11A—C11—H11B	108.5 (13)
C6—C5—C10	122.16 (9)	O2—C12—C11	112.90 (9)
C7—C6—C1	116.51 (9)	O2—C12—H12A	110.5 (9)
C7—C6—C5	123.65 (9)	C11—C12—H12A	108.4 (9)
C1—C6—C5	119.82 (9)	O2—C12—H12B	103.7 (10)
C8—C7—C6	119.89 (9)	C11—C12—H12B	112.3 (10)
C8—C7—H7	121.4 (9)	H12A—C12—H12B	109.1 (13)
C6—C7—H7	118.7 (9)		
C9—N1—C1—C2	178.17 (9)	C4—C5—C6—C7	178.35 (10)
C9—N1—C1—C6	-0.86 (15)	C10—C5—C6—C7	-1.01 (15)
N1—C1—C2—O1	-0.60 (14)	C4—C5—C6—C1	0.05 (14)
C6—C1—C2—O1	178.47 (9)	C10—C5—C6—C1	-179.31 (9)
N1—C1—C2—C3	179.65 (9)	C1—C6—C7—C8	-0.74 (15)
C6—C1—C2—C3	-1.28 (15)	C5—C6—C7—C8	-179.09 (10)
O1—C2—C3—C4	-178.96 (9)	C6—C7—C8—C9	-0.43 (16)
C1—C2—C3—C4	0.80 (15)	C1—N1—C9—C8	-0.44 (16)
C2—C3—C4—C5	0.13 (16)	C7—C8—C9—N1	1.10 (17)
C3—C4—C5—C6	-0.55 (15)	C4—C5—C10—S1	99.16 (10)
C3—C4—C5—C10	178.83 (9)	C6—C5—C10—S1	-81.48 (11)
N1—C1—C6—C7	1.44 (14)	C11—S1—C10—C5	-60.60 (8)
C2—C1—C6—C7	-177.57 (9)	C10—S1—C11—C12	-177.29 (8)
N1—C1—C6—C5	179.86 (9)	S1—C11—C12—O2	63.58 (11)
C2—C1—C6—C5	0.85 (14)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ N1	0.87	2.29	2.7577 (12)	114
O1—H1 $\cdots$ N1 <sup>i</sup>	0.87	2.19	2.8395 (11)	131
O2—H2 $\cdots$ S1 <sup>ii</sup>	0.87	2.47	3.2919 (9)	159
C3—H3 $\cdots$ O1 <sup>iii</sup>	0.955 (16)	2.599 (16)	3.2858 (13)	129.1 (11)
C8—H8 $\cdots$ O2 <sup>iii</sup>	0.903 (17)	2.529 (17)	3.4252 (14)	171.9 (14)
C9—H9 $\cdots$ O1 <sup>i</sup>	0.917 (16)	2.525 (16)	3.0446 (13)	116.3 (12)

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