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## Structure Reports

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## (7-Chloro-2-oxo-2H-chromen-4-yl)-methyl piperidine-1-carbodithioate

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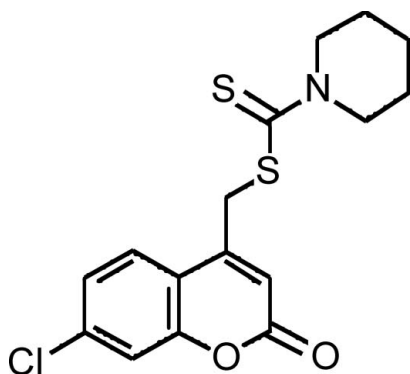
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.082; data-to-parameter ratio = 14.0.

In the title compound,  $\text{C}_{16}\text{H}_{16}\text{ClNO}_2\text{S}_2$ , the piperidine ring is in a chair conformation. In the coumarin ring system, the dihedral angle between the benzene and pyran rings is  $3.5$  (1)°. In the crystal, a weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bond links molecules into chains along [001]. In addition,  $\pi-\pi$  stacking interactions are present involving the benzene and pyran rings, with a centroid-to-centroid distance of  $3.712$  (2) Å. The crystal studied is a nonmerohedral twin with refined components  $0.221$  (1) and  $0.779$  (1).

## Related literature

For structures and properties of coumarins, see: Kulkarni *et al.* (2006); Jones *et al.* (1985); Trenor *et al.* (2004); Hung *et al.* (2007). For the applications of dithiocarbamate compounds, see: Bergendorff & Hansson (2002); Huang *et al.* (2009). For standard bond lengths, see: Allen *et al.* (1987). For ring conformations, see: Duax & Norton (1975). For the synthesis of the title compound, see: Shastri *et al.* (2004); Vasilliev & Polackov (2000).



## Experimental

## Crystal data

$\text{C}_{16}\text{H}_{16}\text{ClNO}_2\text{S}_2$   
 $M_r = 353.87$   
 Monoclinic,  $Pc$   
 $a = 4.9427$  (3) Å  
 $b = 11.5010$  (6) Å  
 $c = 14.0006$  (8) Å  
 $\beta = 90.271$  (6)°  
 $V = 795.87$  (8) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.51$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.3 \times 0.2 \times 0.2$  mm

## Data collection

Oxford Xcalibur Sapphire3 diffractometer  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)  
 $T_{\min} = 0.886$ ,  $T_{\max} = 1.000$   
 13944 measured reflections  
 2801 independent reflections  
 2678 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.082$   
 $S = 1.04$   
 2801 reflections  
 200 parameters  
 2 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.18$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 1394 Friedel pairs  
 Flack parameter:  $-0.01$  (10)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O2}^i$	0.93	2.41	3.167 (5)	139

Symmetry code: (i)  $x - 1, -y + 2, z + \frac{1}{2}$ .

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

KMK is grateful to Karnatak Science College, Dharwad, for providing laboratory facilities. RK acknowledges the Department of Science and Technology for the single-crystal X-ray diffractometer, sanctioned as a National Facility under Project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5420).

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## supporting information

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**(7-Chloro-2-oxo-2H-chromen-4-yl)methyl piperidine-1-carbodithioate**

**K. Mahesh Kumar, Dalbir Kour, Kamini Kapoor, N. M. Mahabaleshwaraiyah, O. Kotresh, Vivek K. Gupta and Rajni Kant**

**S1. Comment**

Coumarins are an important class of heterocycles, which are widespread in the plant kingdom and have been extensively reported. Coumarin derivatives with various substituents at the C-4 position have revealed potential as anti-microbial, anti-viral, anti-oxidant, anti-inflammatory and anti-cancer agents (Kulkarni *et al.*, 2006). They have also found a place and subsequent use in laser dyes, non-linear optical chromophores, fluorescent whiteners, fluorescent probes and solar energy collectors due to their outstanding optical properties (Jones *et al.*, 1985; Trenor *et al.*, 2004; Hung *et al.*, 2007). Dithiocarbamate (DTC) derivatives are valuable compounds due to their interesting chemistry and utility. These compounds have shown wide applications as pesticides, fungicides in agriculture, sulfur vulcanization and anti-cancer agents (Bergendorff & Hansson, 2002; Huang *et al.*, 2009). In our work, we have been able to link a DTC moiety at C-4 methylene carbon and it was a thought of considerable interest to study the effect of this moiety on the total solid-state conformation of the molecule. A new series of piperidine-1-dithiocarbamate derivatives of 4-substituted coumarin was synthesized in a single step and screened for antimicrobial, anti-diabetic, DNA binding and DNA cleavage activity. In this paper we report the crystal structure of (7-Chloro-2-oxo-2H-chromen-4-yl)methyl piperidine-1-carbodithioate (I).

The molecular structure of (I) is shown in Fig. 1. The bond lengths (Allen *et al.*, 1987) and angles in the molecule are within normal ranges. The pyridine ring adopts a normal chair conformation (asymmetry parameters:  $\Delta C_s(C15-N1) = 0.94$ ;  $\Delta C_2(C16-C15) = 2.5$  (Duax & Norton, 1975). The dihedral angle between pyran and benzene rings in the coumarin moiety  $3.5 (1)^\circ$ . In the crystal, weak C—H $\cdots$ O hydrogen bonds link molecules along [001] (Fig. 2). In addition,  $\pi$ – $\pi$  interactions between the pyran ring at  $(x, y, z)$  and the benzene ring at  $(1 + x, y, z)$  are present [centroid separation =  $3.712 (2) \text{ \AA}$ , interplanar spacing =  $3.407 \text{ \AA}$  and centroid shift =  $1.47 \text{ \AA}$ ].

**S2. Experimental**

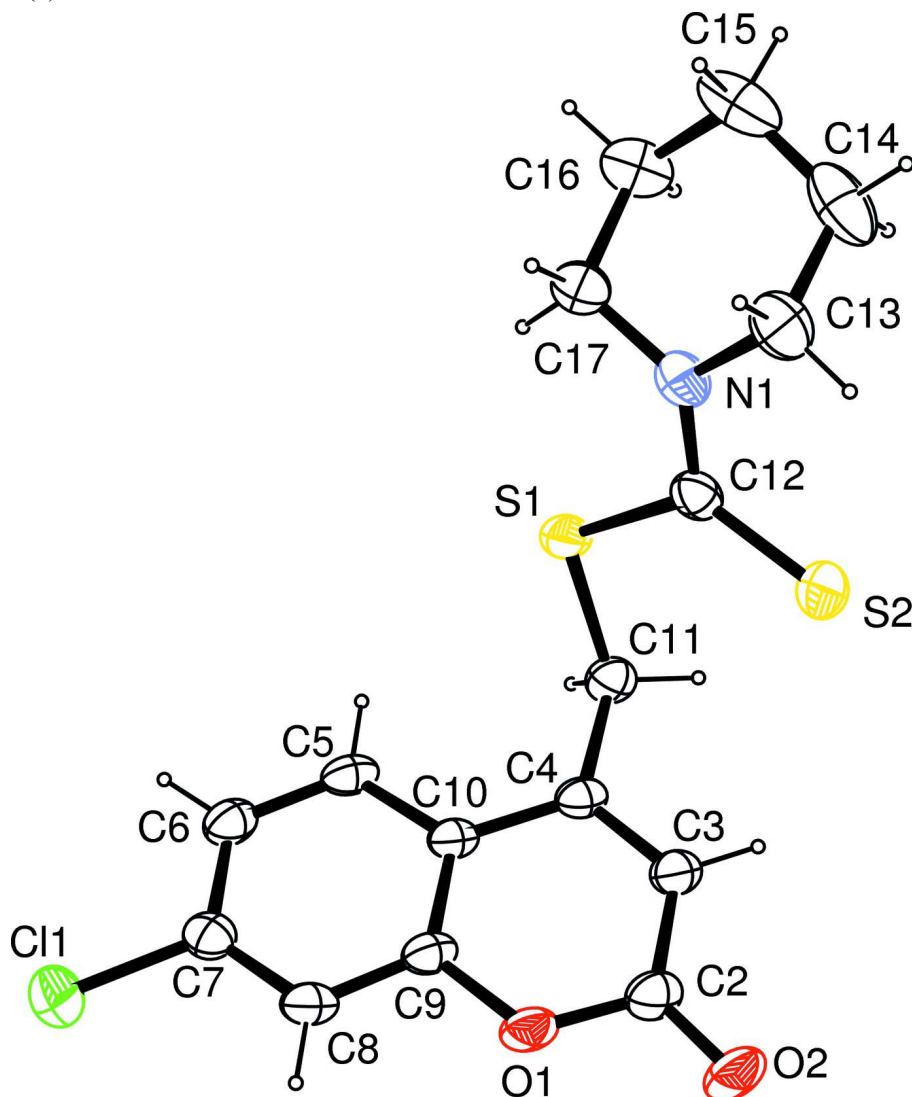
4-Bromomethyl coumarin required for the synthesis of the target molecule was synthesized according to an already reported procedure (Shastri *et al.*, 2004) involving the Pechmann cyclization of phenols with 4-Bromoethyl acetoacetate and the potassium salt of piperidine-1-dithiocarbamate was synthesized according to the procedure reported (Vasilliev & Polackov, 2000).

A mixture of 2.73 g (0.01 mol) of 7-chloro-4-bromomethyl coumarin and 1.99 g (0.01 mol) of potassium salt of piperidine-1-dithiocarbamate in 30 ml dry alcohol was stirred for 12 h at room temperature (the reaction was monitored by TLC). The solvent was evaporated and the solid was extracted twice with MDC–water mixture. The organic solvent was dried over  $\text{CaCl}_2$ , the solvent evaporated and recrystallized from ethanol–chloroform. A slow evaporation technique was used to grow crystals suitable for diffraction studies in an ethanol–chloroform mixture. Yield = 89%, m.p. 407–409 K. IR (KBr): 1720  $\text{cm}^{-1}$  (C=O), 1430  $\text{cm}^{-1}$  (C=S), 849  $\text{cm}^{-1}$  (C–N), 771  $\text{cm}^{-1}$  (C–Cl). GCMS: m/e: 353.03.  $^1\text{H}$  NMR (300 MHz,  $\text{CdCl}_2$ ,  $\delta$ , p.p.m.): 2.81 (s, 4H, C13 & C17–H), 2.79 (s, 6H, C14, C16 & C16–H), 4.72 (s, 2H, C4–CH<sub>2</sub>),

6.21 (s, 1H, C3—H), 7.18 (d, 2H, C6 & C8—H), 7.47 (d, 1H C5—H). Elemental analysis: C, 54.27; H, 4.54; Cl, 10.00; N, 3.92; O, 9.01; S, 18.09.

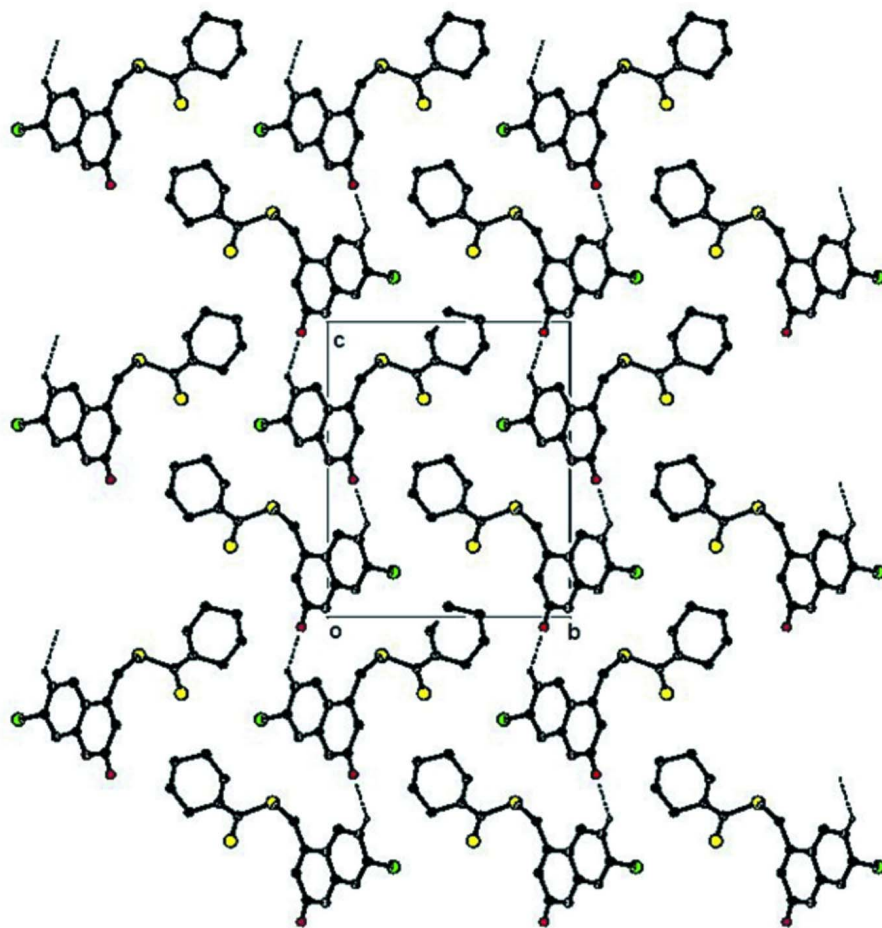
### S3. Refinement

All H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93–0.97 Å and with  $U_{iso}(H) = 1.2U_{eq}(C)$ . The crystal studied is a non-merohedral twin with refined components 0.221 (1) and 0.779 (1) and twin law 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 -1.00.



**Figure 1**

The molecular structure of the title compound. Ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

The packing arrangement of molecules viewed along the *a* axis. The broken lines show the intermolecular C—H...O interactions.

**(7-Chloro-2-oxo-2*H*-chromen-4-yl)methyl piperidine-1-carbodithioate**

*Crystal data*

$C_{16}H_{16}ClNO_2S_2$

$M_r = 353.87$

Monoclinic, *Pc*

Hall symbol: *p* -2yc

$a = 4.9427$  (3) Å

$b = 11.5010$  (6) Å

$c = 14.0006$  (8) Å

$\beta = 90.271$  (6)°

$V = 795.87$  (8) Å<sup>3</sup>

$Z = 2$

$F(000) = 368$

$D_x = 1.477$  Mg m<sup>-3</sup>

Mo *K*α radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7572 reflections

$\theta = 3.4$ – $29.0$ °

$\mu = 0.51$  mm<sup>-1</sup>

$T = 293$  K

Block, white

$0.3 \times 0.2 \times 0.2$  mm

*Data collection*

Oxford Xcalibur Sapphire3

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.1049 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2010)

$T_{\min} = 0.886$ ,  $T_{\max} = 1.000$   
 13944 measured reflections  
 2801 independent reflections  
 2678 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -5 \rightarrow 5$   
 $k = -13 \rightarrow 13$   
 $l = -16 \rightarrow 16$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.082$   
 $S = 1.04$   
 2801 reflections  
 200 parameters  
 2 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.3317P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.14 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: Flack (1983), with 1394  
 Friedel pairs  
 Absolute structure parameter:  $-0.01 (10)$

*Special details*

**Experimental.** CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171.NET) (compiled Aug 27 2010, 11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.1990 (2)	0.77560 (7)	0.36977 (7)	0.0421 (3)
S2	0.4685 (3)	0.60142 (9)	0.24062 (9)	0.0525 (3)
Cl1	-0.4816 (2)	1.27262 (9)	0.15209 (9)	0.0577 (3)
O1	0.2148 (6)	0.9922 (2)	0.03114 (17)	0.0429 (7)
C2	0.4260 (9)	0.9155 (3)	0.0384 (3)	0.0431 (10)
O2	0.5440 (8)	0.8931 (3)	-0.03402 (19)	0.0583 (9)
C3	0.4925 (9)	0.8712 (3)	0.1330 (3)	0.0373 (9)
H3	0.6290	0.8161	0.1393	0.045*
C4	0.3622 (8)	0.9077 (3)	0.2120 (2)	0.0328 (8)
C10	0.1525 (8)	0.9952 (3)	0.2026 (2)	0.0315 (8)
C5	0.0142 (9)	1.0460 (3)	0.2788 (2)	0.0362 (8)
H5	0.0531	1.0225	0.3410	0.043*
C6	-0.1802 (9)	1.1309 (3)	0.2633 (3)	0.0405 (10)
H6	-0.2696	1.1644	0.3147	0.049*
C7	-0.2409 (8)	1.1657 (3)	0.1707 (3)	0.0372 (9)
C8	-0.1117 (9)	1.1168 (3)	0.0933 (3)	0.0385 (9)

H8	-0.1538	1.1396	0.0313	0.046*
C9	0.0813 (8)	1.0334 (3)	0.1108 (2)	0.0354 (9)
C11	0.4485 (9)	0.8620 (3)	0.3081 (3)	0.0382 (9)
H11B	0.4967	0.9276	0.3484	0.046*
H11A	0.6100	0.8153	0.2998	0.046*
C12	0.2473 (9)	0.6313 (3)	0.3254 (3)	0.0378 (9)
N1	0.0894 (7)	0.5538 (3)	0.3692 (3)	0.0487 (9)
C17	-0.0804 (10)	0.5754 (4)	0.4518 (4)	0.0538 (12)
H17A	-0.2672	0.5577	0.4360	0.065*
H17B	-0.0697	0.6569	0.4694	0.065*
C16	0.0100 (13)	0.5010 (4)	0.5353 (4)	0.0637 (12)
H16A	-0.1126	0.5127	0.5884	0.076*
H16B	0.1891	0.5253	0.5557	0.076*
C15	0.0164 (14)	0.3726 (4)	0.5096 (4)	0.0732 (16)
H15A	-0.1668	0.3446	0.4997	0.088*
H15B	0.0962	0.3287	0.5618	0.088*
C14	0.1810 (12)	0.3540 (4)	0.4192 (4)	0.0719 (17)
H14B	0.3697	0.3712	0.4323	0.086*
H14A	0.1684	0.2731	0.4000	0.086*
C13	0.0825 (11)	0.4303 (3)	0.3383 (4)	0.0609 (14)
H13A	0.1971	0.4198	0.2829	0.073*
H13B	-0.1008	0.4087	0.3207	0.073*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0626 (7)	0.0293 (5)	0.0344 (5)	0.0036 (5)	0.0134 (5)	0.0018 (4)
S2	0.0701 (7)	0.0446 (6)	0.0429 (5)	0.0132 (5)	0.0119 (6)	-0.0038 (5)
Cl1	0.0600 (7)	0.0446 (6)	0.0686 (8)	0.0118 (5)	0.0082 (6)	0.0067 (5)
O1	0.0627 (18)	0.0443 (16)	0.0218 (12)	0.0010 (14)	0.0080 (13)	-0.0001 (11)
C2	0.064 (3)	0.0350 (19)	0.031 (2)	-0.003 (2)	0.0083 (19)	-0.0062 (16)
O2	0.083 (2)	0.0600 (19)	0.0322 (16)	0.0051 (18)	0.0230 (17)	-0.0058 (13)
C3	0.048 (2)	0.0316 (18)	0.0324 (19)	-0.0030 (18)	0.0071 (19)	-0.0001 (15)
C4	0.041 (2)	0.0289 (18)	0.0287 (19)	-0.0076 (15)	0.0040 (15)	0.0011 (14)
C10	0.040 (2)	0.0283 (18)	0.0258 (19)	-0.0056 (16)	0.0035 (15)	0.0010 (14)
C5	0.050 (2)	0.0362 (19)	0.0224 (17)	-0.0096 (19)	0.0046 (16)	-0.0007 (14)
C6	0.053 (3)	0.034 (2)	0.035 (2)	-0.0039 (18)	0.0123 (18)	-0.0036 (16)
C7	0.040 (2)	0.0297 (19)	0.042 (2)	-0.0062 (16)	0.0032 (18)	0.0033 (16)
C8	0.051 (3)	0.034 (2)	0.0305 (19)	-0.0055 (18)	0.0035 (18)	0.0056 (16)
C9	0.050 (2)	0.0311 (18)	0.0255 (18)	-0.0070 (17)	0.0069 (16)	-0.0014 (14)
C11	0.050 (3)	0.0372 (18)	0.0272 (19)	0.0007 (18)	0.0024 (17)	-0.0029 (16)
C12	0.049 (2)	0.034 (2)	0.0302 (19)	0.0047 (18)	-0.0042 (18)	0.0013 (15)
N1	0.061 (2)	0.0286 (16)	0.056 (2)	0.0022 (15)	0.006 (2)	0.0004 (15)
C17	0.060 (3)	0.037 (2)	0.064 (3)	-0.001 (2)	0.013 (2)	0.009 (2)
C16	0.076 (3)	0.055 (3)	0.060 (3)	-0.005 (3)	-0.005 (3)	0.012 (2)
C15	0.087 (4)	0.044 (2)	0.088 (4)	-0.011 (3)	-0.029 (4)	0.023 (3)
C14	0.070 (4)	0.034 (2)	0.112 (5)	0.001 (2)	-0.028 (4)	-0.003 (3)
C13	0.077 (4)	0.031 (2)	0.075 (3)	-0.003 (2)	0.006 (3)	-0.008 (2)

*Geometric parameters (Å, °)*

S1—C12	1.788 (4)	C8—H8	0.9300
S1—C11	1.807 (4)	C11—H11B	0.9700
S2—C12	1.654 (4)	C11—H11A	0.9700
C11—C7	1.730 (4)	C12—N1	1.336 (5)
O1—C2	1.371 (5)	N1—C17	1.454 (5)
O1—C9	1.382 (4)	N1—C13	1.485 (5)
C2—O2	1.200 (4)	C17—C16	1.514 (6)
C2—C3	1.456 (5)	C17—H17A	0.9700
C3—C4	1.349 (5)	C17—H17B	0.9700
C3—H3	0.9300	C16—C15	1.521 (7)
C4—C10	1.450 (5)	C16—H16A	0.9700
C4—C11	1.505 (5)	C16—H16B	0.9700
C10—C5	1.398 (5)	C15—C14	1.524 (8)
C10—C9	1.402 (5)	C15—H15A	0.9700
C5—C6	1.386 (6)	C15—H15B	0.9700
C5—H5	0.9300	C14—C13	1.511 (7)
C6—C7	1.388 (5)	C14—H14B	0.9700
C6—H6	0.9300	C14—H14A	0.9700
C7—C8	1.380 (6)	C13—H13A	0.9700
C8—C9	1.374 (6)	C13—H13B	0.9700
C12—S1—C11	104.60 (18)	N1—C12—S1	112.4 (3)
C2—O1—C9	121.8 (3)	S2—C12—S1	122.2 (2)
O2—C2—O1	116.7 (4)	C12—N1—C17	126.3 (3)
O2—C2—C3	125.9 (4)	C12—N1—C13	121.2 (4)
O1—C2—C3	117.5 (3)	C17—N1—C13	112.5 (4)
C4—C3—C2	122.1 (4)	N1—C17—C16	110.4 (4)
C4—C3—H3	119.0	N1—C17—H17A	109.6
C2—C3—H3	119.0	C16—C17—H17A	109.6
C3—C4—C10	119.1 (3)	N1—C17—H17B	109.6
C3—C4—C11	119.3 (4)	C16—C17—H17B	109.6
C10—C4—C11	121.5 (3)	H17A—C17—H17B	108.1
C5—C10—C9	116.6 (3)	C17—C16—C15	111.8 (5)
C5—C10—C4	125.0 (3)	C17—C16—H16A	109.2
C9—C10—C4	118.5 (3)	C15—C16—H16A	109.2
C6—C5—C10	121.0 (3)	C17—C16—H16B	109.2
C6—C5—H5	119.5	C15—C16—H16B	109.2
C10—C5—H5	119.5	H16A—C16—H16B	107.9
C5—C6—C7	119.8 (4)	C16—C15—C14	110.2 (4)
C5—C6—H6	120.1	C16—C15—H15A	109.6
C7—C6—H6	120.1	C14—C15—H15A	109.6
C8—C7—C6	121.1 (4)	C16—C15—H15B	109.6
C8—C7—C11	119.5 (3)	C14—C15—H15B	109.6
C6—C7—C11	119.4 (3)	H15A—C15—H15B	108.1
C9—C8—C7	117.9 (4)	C13—C14—C15	111.7 (5)
C9—C8—H8	121.0	C13—C14—H14B	109.3



C7—C8—H8	121.0	C15—C14—H14B	109.3
C8—C9—O1	115.4 (3)	C13—C14—H14A	109.3
C8—C9—C10	123.6 (3)	C15—C14—H14A	109.3
O1—C9—C10	120.9 (3)	H14B—C14—H14A	107.9
C4—C11—S1	115.4 (3)	N1—C13—C14	109.3 (4)
C4—C11—H11B	108.4	N1—C13—H13A	109.8
S1—C11—H11B	108.4	C14—C13—H13A	109.8
C4—C11—H11A	108.4	N1—C13—H13B	109.8
S1—C11—H11A	108.4	C14—C13—H13B	109.8
H11B—C11—H11A	107.5	H13A—C13—H13B	108.3
N1—C12—S2	125.5 (3)		
C9—O1—C2—O2	-173.5 (4)	C5—C10—C9—C8	0.5 (5)
C9—O1—C2—C3	4.7 (5)	C4—C10—C9—C8	-179.1 (4)
O2—C2—C3—C4	174.8 (4)	C5—C10—C9—O1	177.1 (3)
O1—C2—C3—C4	-3.2 (6)	C4—C10—C9—O1	-2.5 (5)
C2—C3—C4—C10	-1.1 (6)	C3—C4—C11—S1	-115.6 (4)
C2—C3—C4—C11	-177.6 (4)	C10—C4—C11—S1	68.0 (4)
C3—C4—C10—C5	-175.7 (4)	C12—S1—C11—C4	86.3 (3)
C11—C4—C10—C5	0.7 (5)	C11—S1—C12—N1	175.5 (3)
C3—C4—C10—C9	3.9 (5)	C11—S1—C12—S2	-3.6 (3)
C11—C4—C10—C9	-179.7 (3)	S2—C12—N1—C17	171.5 (4)
C9—C10—C5—C6	-0.9 (5)	S1—C12—N1—C17	-7.6 (5)
C4—C10—C5—C6	178.7 (4)	S2—C12—N1—C13	-5.4 (6)
C10—C5—C6—C7	0.5 (6)	S1—C12—N1—C13	175.4 (3)
C5—C6—C7—C8	0.3 (6)	C12—N1—C17—C16	-117.9 (5)
C5—C6—C7—C11	-179.4 (3)	C13—N1—C17—C16	59.3 (5)
C6—C7—C8—C9	-0.7 (6)	N1—C17—C16—C15	-55.2 (6)
C11—C7—C8—C9	179.0 (3)	C17—C16—C15—C14	52.2 (7)
C7—C8—C9—O1	-176.5 (3)	C16—C15—C14—C13	-53.3 (6)
C7—C8—C9—C10	0.3 (6)	C12—N1—C13—C14	117.5 (5)
C2—O1—C9—C8	175.0 (3)	C17—N1—C13—C14	-59.8 (6)
C2—O1—C9—C10	-1.9 (5)	C15—C14—C13—N1	56.3 (6)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C17—H17B $\cdots$ S1	0.97	2.36	2.923 (5)	116
C13—H13A $\cdots$ S2	0.97	2.55	3.067 (4)	113
C6—H6 $\cdots$ O2 <sup>i</sup>	0.93	2.41	3.167 (5)	139

Symmetry code: (i)  $x-1, -y+2, z+1/2$ .