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# (5,7-Dimethyl-2-oxo-2H-chromen-4-yl)methyl morpholine-4-carbodithioate

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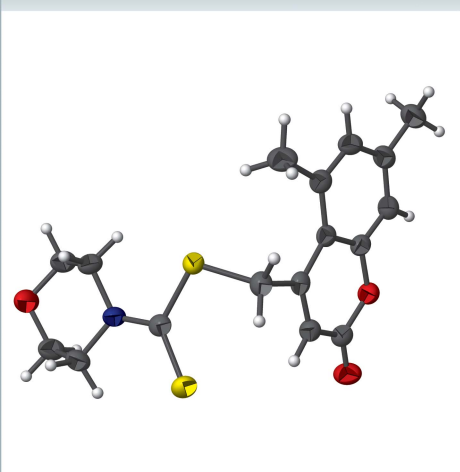
**Keywords:** crystal structure; inversion dimers; hydrogen bonds; 2H-chromene; morpholine-4-carbodithioate ester.

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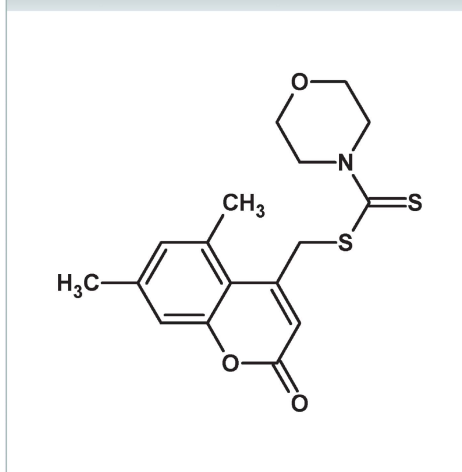
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>17</sub>H<sub>19</sub>NO<sub>3</sub>S<sub>2</sub>, the 2H-chromene ring system is nearly planar, with a maximum deviation of 0.080 (2) Å, and the morpholine ring adopts a chair conformation. The bond-angle sum at the N atom is 358°. The coumarin unit makes dihedral angle of 86.34 (9)° with the morpholine ring. A short intramolecular C—H···S contact generates an S(7) ring. In the crystal, inversion dimers linked by pairs of weak C—H···O hydrogen bonds generate R<sub>2</sub><sup>2</sup>(16) loops. Aromatic π–π interactions [shortest centroid–centroid distance = 3.8599 (13) Å] also occur.

## 3D view



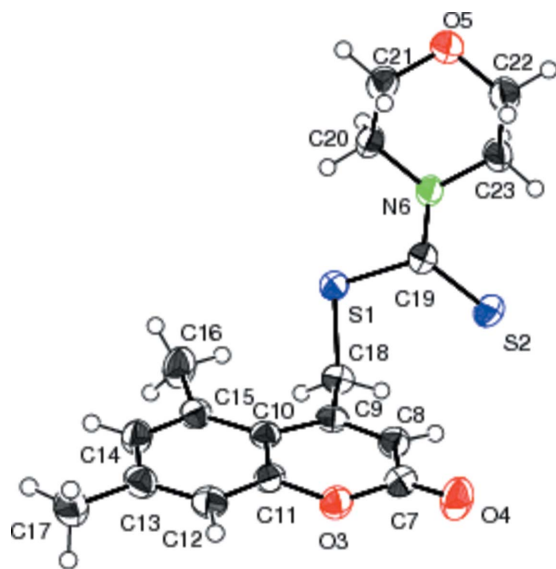
## Chemical scheme



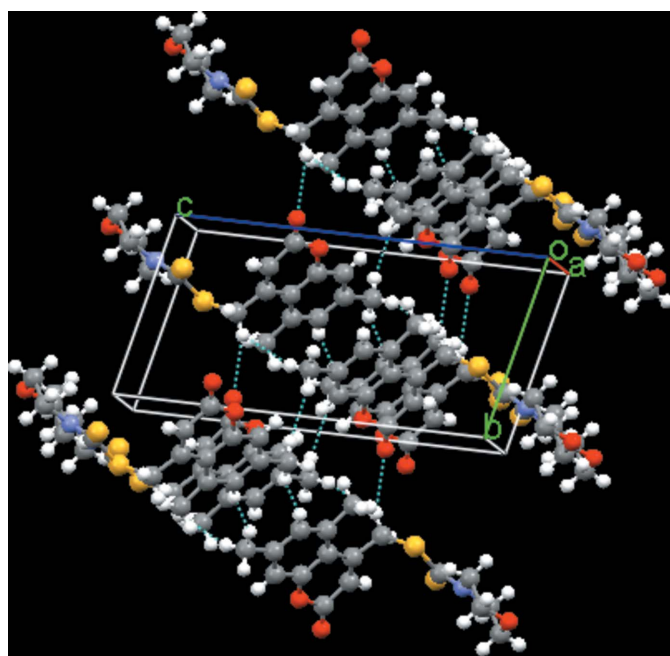
## Structure description

Recently, dithiocarbamic acid esters, a common class of organic molecules, have also attracted attention due to their anti-cancer action (Scozzafava *et al.*, 2000) in derivatives such as thalidomide dithiocarbamates (Zahran *et al.*, 2008) and chromone dithiocarbamates (Huang *et al.*, 2009). As part of our studies in this area, we now describe the structure of the title compound (Kant *et al.*, 2012).

The asymmetric unit is shown in Fig. 1. The 2H-chromene ring systems is nearly planar, with a maximum deviation of 0.0804 (22) Å for the atom C7 and the morpholine ring adopts a chair conformation. The coumarin unit makes dihedral angle of 86.34 (9)° with morpholine ring. In the crystal, C—H···O hydrogen bonds (Table 1, Fig. 2) and π–π interactions between fused benzene rings of chromene [shortest centroid–centroid distance = 3.8599 (13) Å] are observed.



**Figure 1**  
Perspective diagram of the title molecule drawn with 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radius.



**Figure 2**  
Packing diagram of the molecule viewed parallel to the *b* axis.

### Synthesis and crystallization

This compound was prepared according to the reported method (Kant *et al.*, 2012). Colourless needles of the title compound were grown from a mixed solution of EtOH/CHCl<sub>3</sub> (*v/v* = 1/1) by slow evaporation at room temperature. Yield = 81%, m.p. 445 K. IR (KBr): 645 cm<sup>-1</sup>(C–S), 1231 cm<sup>-1</sup> (C=S), 1039 cm<sup>-1</sup>(C–O), 850 cm<sup>-1</sup> (C–N), 1118 cm<sup>-1</sup>(C–O–C), 1711 cm<sup>-1</sup>(C=O). GCMS: *m/e*: 349. 1H NMR (400 MHz, CDCl<sub>3</sub>, δ, p.p.m.) 2.21 (*t*, 3H, –CH<sub>3</sub>), 2.61 (*t*, 3H, –CH<sub>3</sub>), 3.61 (*s*, 4H, morpholine-CH<sub>2</sub>), 3.80 (*s*, 2H, morpholine-

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

<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>
C16–H16C···S1	0.96	2.62	3.358 (2)	134
C17–H17A···O4 <sup>i</sup>	0.96	2.58	3.505 (2)	162

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>17</sub> H <sub>19</sub> NO <sub>3</sub> S <sub>2</sub>
<i>M<sub>r</sub></i>	349.45
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.9573 (2), 7.9838 (2), 15.6037 (4)
$\alpha$ , $\beta$ , $\gamma$ (°)	75.485 (2), 87.122 (1), 75.763 (1)
<i>V</i> (Å <sup>3</sup> )	813.22 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.34
Crystal size (mm)	0.24 × 0.20 × 0.12
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2009)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.770, 1.000
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	12588, 2857, 2551
<i>R<sub>int</sub></i>	0.036
(sin $\theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.595
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.030, 0.084, 1.08
No. of reflections	2857
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.20, –0.20

Computer programs: *SMART* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012).

CH<sub>2</sub>), 4.15(*s*, 2H, morpholine-CH<sub>2</sub>), 4.65 (*t*, 2H, Methylene-CH<sub>2</sub>), 6.33 (*s*, 1H, Ar–H), 6.77 (*s*, 1H, Ar–H), 6.84 (*s*, 1H, Ar–H). Elemental analysis for C<sub>17</sub>H<sub>19</sub>NO<sub>3</sub>S<sub>2</sub>: C, 58.37; H, 5.42; N, 3.91.

### 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**, x160169 [https://doi.org/10.1107/S2414314616001693]

(5,7-Dimethyl-2-oxo-2*H*-chromen-4-yl)methyl morpholine-4-carbodithioate

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(5,7-Dimethyl-2-oxo-2*H*-chromen-4-yl)methyl morpholine-4-carbodithioate*Crystal data*

$C_{17}H_{19}NO_3S_2$	$F(000) = 368$
$M_r = 349.45$	$D_x = 1.427 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Melting point: 445 K
$a = 6.9573 (2) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 7.9838 (2) \text{ \AA}$	Cell parameters from 2857 reflections
$c = 15.6037 (4) \text{ \AA}$	$\theta = 1.4\text{--}25.0^\circ$
$\alpha = 75.485 (2)^\circ$	$\mu = 0.34 \text{ mm}^{-1}$
$\beta = 87.122 (1)^\circ$	$T = 296 \text{ K}$
$\gamma = 75.763 (1)^\circ$	Plate, colourless
$V = 813.22 (4) \text{ \AA}^3$	$0.24 \times 0.20 \times 0.12 \text{ mm}$
$Z = 2$	

*Data collection*

Bruker SMART CCD area-detector diffractometer	12588 measured reflections
Radiation source: fine-focus sealed tube	2857 independent reflections
Graphite monochromator	2551 reflections with $I > 2\sigma(I)$
$\omega$ and $\phi$ scans	$R_{\text{int}} = 0.036$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 1.4^\circ$
$T_{\text{min}} = 0.770$ , $T_{\text{max}} = 1.000$	$h = -8 \rightarrow 8$
	$k = -9 \rightarrow 9$
	$l = -18 \rightarrow 18$

*Refinement*

Refinement on $F^2$	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.1658P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
2857 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
211 parameters	Extinction correction: SHELXL2014 (Sheldrick, 2015),
0 restraints	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Hydrogen site location: inferred from neighbouring sites	Extinction coefficient: 0.041 (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.

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	0.69951 (6)	0.57313 (5)	0.12898 (2)	0.03649 (15)
S2	1.06731 (6)	0.70892 (6)	0.06881 (3)	0.04197 (15)
O5	0.54406 (19)	0.92765 (17)	-0.19357 (8)	0.0492 (3)
O3	0.65176 (17)	0.93171 (14)	0.37562 (7)	0.0371 (3)
O4	0.8819 (2)	1.05956 (16)	0.30663 (9)	0.0512 (3)
N6	0.74909 (19)	0.75809 (17)	-0.03019 (8)	0.0328 (3)
C7	0.8041 (3)	0.9362 (2)	0.31725 (10)	0.0367 (4)
C8	0.8592 (2)	0.7900 (2)	0.27620 (10)	0.0352 (4)
H8	0.9736	0.7805	0.2425	0.042*
C9	0.7553 (2)	0.66529 (19)	0.28349 (9)	0.0307 (3)
C10	0.5788 (2)	0.67346 (19)	0.33885 (9)	0.0303 (3)
C11	0.5375 (2)	0.80899 (19)	0.38456 (9)	0.0320 (3)
C12	0.3827 (3)	0.8326 (2)	0.44271 (10)	0.0379 (4)
H12	0.3637	0.9241	0.4716	0.045*
C13	0.2570 (3)	0.7202 (2)	0.45765 (10)	0.0385 (4)
C17	0.0869 (3)	0.7390 (3)	0.52080 (12)	0.0503 (5)
H17A	0.1041	0.8149	0.5573	0.076*
H17B	0.0833	0.6237	0.5575	0.076*
H17C	-0.0353	0.7904	0.4879	0.076*
C14	0.2918 (3)	0.5867 (2)	0.41183 (11)	0.0393 (4)
H14	0.2060	0.5112	0.4210	0.047*
C15	0.4458 (2)	0.5596 (2)	0.35363 (10)	0.0354 (4)
C16	0.4565 (3)	0.4090 (2)	0.30953 (13)	0.0523 (5)
H16A	0.3469	0.3558	0.3282	0.078*
H16B	0.5787	0.3208	0.3260	0.078*
H16C	0.4507	0.4549	0.2464	0.078*
C18	0.8329 (2)	0.5257 (2)	0.23235 (10)	0.0347 (4)
H18A	0.8219	0.4104	0.2684	0.042*
H18B	0.9723	0.5194	0.2201	0.042*
C19	0.8421 (2)	0.69039 (19)	0.04831 (10)	0.0306 (3)
C20	0.5643 (2)	0.7179 (2)	-0.05154 (11)	0.0390 (4)
H20A	0.4905	0.6889	0.0023	0.047*
H20B	0.5961	0.6148	-0.0765	0.047*
C21	0.4390 (3)	0.8729 (2)	-0.11608 (11)	0.0432 (4)
H21A	0.3226	0.8400	-0.1318	0.052*
H21B	0.3945	0.9717	-0.0884	0.052*
C22	0.7086 (3)	0.9846 (2)	-0.17124 (12)	0.0459 (4)
H22A	0.6613	1.0835	-0.1439	0.055*
H22B	0.7775	1.0267	-0.2249	0.055*
C23	0.8509 (3)	0.8381 (2)	-0.10910 (11)	0.0403 (4)
H23A	0.9138	0.7468	-0.1394	0.048*
H23B	0.9537	0.8855	-0.0911	0.048*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0415 (3)	0.0421 (2)	0.0314 (2)	-0.0195 (2)	0.00148 (17)	-0.00998 (16)
S2	0.0293 (2)	0.0542 (3)	0.0440 (3)	-0.0129 (2)	-0.00102 (18)	-0.01193 (19)
O5	0.0426 (7)	0.0605 (8)	0.0402 (6)	-0.0188 (6)	-0.0063 (5)	0.0033 (5)
O3	0.0413 (7)	0.0378 (6)	0.0383 (6)	-0.0148 (5)	0.0040 (5)	-0.0160 (5)
O4	0.0559 (8)	0.0475 (7)	0.0639 (8)	-0.0285 (7)	0.0133 (6)	-0.0251 (6)
N6	0.0277 (7)	0.0347 (7)	0.0355 (7)	-0.0102 (6)	0.0002 (5)	-0.0055 (5)
C7	0.0368 (9)	0.0392 (9)	0.0369 (8)	-0.0124 (8)	-0.0012 (7)	-0.0110 (7)
C8	0.0344 (9)	0.0395 (9)	0.0342 (8)	-0.0105 (7)	0.0020 (7)	-0.0123 (6)
C9	0.0335 (8)	0.0290 (7)	0.0267 (7)	-0.0031 (7)	-0.0051 (6)	-0.0050 (6)
C10	0.0327 (8)	0.0293 (7)	0.0271 (7)	-0.0064 (7)	-0.0046 (6)	-0.0034 (6)
C11	0.0341 (9)	0.0305 (8)	0.0315 (8)	-0.0089 (7)	-0.0040 (6)	-0.0060 (6)
C12	0.0408 (10)	0.0385 (9)	0.0349 (8)	-0.0074 (8)	0.0010 (7)	-0.0120 (7)
C13	0.0348 (9)	0.0421 (9)	0.0340 (8)	-0.0062 (8)	-0.0001 (7)	-0.0037 (7)
C17	0.0442 (11)	0.0601 (11)	0.0456 (10)	-0.0145 (9)	0.0088 (8)	-0.0109 (8)
C14	0.0377 (9)	0.0397 (9)	0.0410 (9)	-0.0157 (8)	-0.0009 (7)	-0.0041 (7)
C15	0.0395 (9)	0.0317 (8)	0.0342 (8)	-0.0092 (7)	-0.0039 (7)	-0.0052 (6)
C16	0.0590 (13)	0.0466 (10)	0.0644 (12)	-0.0286 (10)	0.0127 (10)	-0.0243 (9)
C18	0.0379 (9)	0.0315 (8)	0.0336 (8)	-0.0053 (7)	-0.0017 (7)	-0.0087 (6)
C19	0.0305 (8)	0.0266 (7)	0.0356 (8)	-0.0046 (6)	0.0019 (6)	-0.0116 (6)
C20	0.0355 (9)	0.0408 (9)	0.0418 (9)	-0.0164 (8)	-0.0035 (7)	-0.0042 (7)
C21	0.0319 (9)	0.0474 (10)	0.0468 (9)	-0.0107 (8)	-0.0033 (7)	-0.0035 (8)
C22	0.0417 (10)	0.0463 (10)	0.0464 (10)	-0.0170 (8)	-0.0005 (8)	0.0010 (8)
C23	0.0327 (9)	0.0468 (9)	0.0384 (9)	-0.0114 (8)	0.0042 (7)	-0.0039 (7)

*Geometric parameters (Å, °)*

S1—C19	1.7850 (15)	C13—C17	1.505 (2)
S1—C18	1.8104 (16)	C17—H17A	0.9600
S2—C19	1.6634 (16)	C17—H17B	0.9600
O5—C21	1.411 (2)	C17—H17C	0.9600
O5—C22	1.419 (2)	C14—C15	1.381 (2)
O3—C7	1.3636 (19)	C14—H14	0.9300
O3—C11	1.3837 (18)	C15—C16	1.513 (2)
O4—C7	1.2088 (19)	C16—H16A	0.9600
N6—C19	1.337 (2)	C16—H16B	0.9600
N6—C23	1.472 (2)	C16—H16C	0.9600
N6—C20	1.472 (2)	C18—H18A	0.9700
C7—C8	1.432 (2)	C18—H18B	0.9700
C8—C9	1.347 (2)	C20—C21	1.497 (2)
C8—H8	0.9300	C20—H20A	0.9700
C9—C10	1.463 (2)	C20—H20B	0.9700
C9—C18	1.509 (2)	C21—H21A	0.9700
C10—C11	1.406 (2)	C21—H21B	0.9700
C10—C15	1.422 (2)	C22—C23	1.499 (2)
C11—C12	1.381 (2)	C22—H22A	0.9700

C12—C13	1.373 (2)	C22—H22B	0.9700
C12—H12	0.9300	C23—H23A	0.9700
C13—C14	1.394 (2)	C23—H23B	0.9700
C19—S1—C18	104.75 (7)	C15—C16—H16A	109.5
C21—O5—C22	109.33 (13)	C15—C16—H16B	109.5
C7—O3—C11	121.95 (12)	H16A—C16—H16B	109.5
C19—N6—C23	121.25 (13)	C15—C16—H16C	109.5
C19—N6—C20	123.64 (13)	H16A—C16—H16C	109.5
C23—N6—C20	113.10 (13)	H16B—C16—H16C	109.5
O4—C7—O3	117.53 (14)	C9—C18—S1	112.31 (10)
O4—C7—C8	126.46 (16)	C9—C18—H18A	109.1
O3—C7—C8	115.98 (14)	S1—C18—H18A	109.1
C9—C8—C7	123.98 (15)	C9—C18—H18B	109.1
C9—C8—H8	118.0	S1—C18—H18B	109.1
C7—C8—H8	118.0	H18A—C18—H18B	107.9
C8—C9—C10	119.08 (14)	N6—C19—S2	124.20 (12)
C8—C9—C18	116.07 (14)	N6—C19—S1	112.43 (11)
C10—C9—C18	124.85 (13)	S2—C19—S1	123.36 (9)
C11—C10—C15	115.86 (14)	N6—C20—C21	111.12 (13)
C11—C10—C9	115.87 (13)	N6—C20—H20A	109.4
C15—C10—C9	128.26 (14)	C21—C20—H20A	109.4
C12—C11—O3	113.45 (13)	N6—C20—H20B	109.4
C12—C11—C10	124.13 (14)	C21—C20—H20B	109.4
O3—C11—C10	122.42 (14)	H20A—C20—H20B	108.0
C13—C12—C11	119.55 (15)	O5—C21—C20	111.68 (14)
C13—C12—H12	120.2	O5—C21—H21A	109.3
C11—C12—H12	120.2	C20—C21—H21A	109.3
C12—C13—C14	117.62 (15)	O5—C21—H21B	109.3
C12—C13—C17	121.79 (16)	C20—C21—H21B	109.3
C14—C13—C17	120.59 (16)	H21A—C21—H21B	107.9
C13—C17—H17A	109.5	O5—C22—C23	112.16 (14)
C13—C17—H17B	109.5	O5—C22—H22A	109.2
H17A—C17—H17B	109.5	C23—C22—H22A	109.2
C13—C17—H17C	109.5	O5—C22—H22B	109.2
H17A—C17—H17C	109.5	C23—C22—H22B	109.2
H17B—C17—H17C	109.5	H22A—C22—H22B	107.9
C15—C14—C13	124.03 (15)	N6—C23—C22	111.21 (14)
C15—C14—H14	118.0	N6—C23—H23A	109.4
C13—C14—H14	118.0	C22—C23—H23A	109.4
C14—C15—C10	118.78 (15)	N6—C23—H23B	109.4
C14—C15—C16	115.96 (15)	C22—C23—H23B	109.4
C10—C15—C16	125.25 (15)	H23A—C23—H23B	108.0
C11—O3—C7—O4	172.02 (14)	C13—C14—C15—C16	-179.20 (16)
C11—O3—C7—C8	-9.6 (2)	C11—C10—C15—C14	-1.4 (2)
O4—C7—C8—C9	-173.11 (16)	C9—C10—C15—C14	177.29 (14)
O3—C7—C8—C9	8.7 (2)	C11—C10—C15—C16	177.88 (15)

C7—C8—C9—C10	-2.2 (2)	C9—C10—C15—C16	-3.5 (3)
C7—C8—C9—C18	177.64 (14)	C8—C9—C18—S1	-99.37 (15)
C8—C9—C10—C11	-3.3 (2)	C10—C9—C18—S1	80.51 (16)
C18—C9—C10—C11	176.86 (13)	C19—S1—C18—C9	94.28 (12)
C8—C9—C10—C15	178.07 (14)	C23—N6—C19—S2	7.4 (2)
C18—C9—C10—C15	-1.8 (2)	C20—N6—C19—S2	170.20 (12)
C7—O3—C11—C12	-176.06 (13)	C23—N6—C19—S1	-171.43 (11)
C7—O3—C11—C10	4.5 (2)	C20—N6—C19—S1	-8.65 (19)
C15—C10—C11—C12	1.7 (2)	C18—S1—C19—N6	-171.04 (11)
C9—C10—C11—C12	-177.11 (14)	C18—S1—C19—S2	10.10 (12)
C15—C10—C11—O3	-178.87 (13)	C19—N6—C20—C21	148.50 (15)
C9—C10—C11—O3	2.3 (2)	C23—N6—C20—C21	-47.48 (19)
O3—C11—C12—C13	179.83 (14)	C22—O5—C21—C20	-61.97 (19)
C10—C11—C12—C13	-0.7 (2)	N6—C20—C21—O5	55.36 (19)
C11—C12—C13—C14	-0.6 (2)	C21—O5—C22—C23	61.16 (19)
C11—C12—C13—C17	179.55 (15)	C19—N6—C23—C22	-148.99 (15)
C12—C13—C14—C15	0.9 (3)	C20—N6—C23—C22	46.56 (19)
C17—C13—C14—C15	-179.25 (15)	O5—C22—C23—N6	-53.5 (2)
C13—C14—C15—C10	0.1 (2)		

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C16—H16C...S1	0.96	2.62	3.358 (2)	134
C17—H17A...O4 <sup>i</sup>	0.96	2.58	3.505 (2)	162

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