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(7, 8-Dimethyl-2-oxo-2*H*-chromen-4-yl)methyl morpholine-4-carbodithioate

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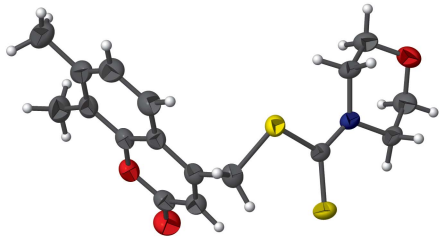
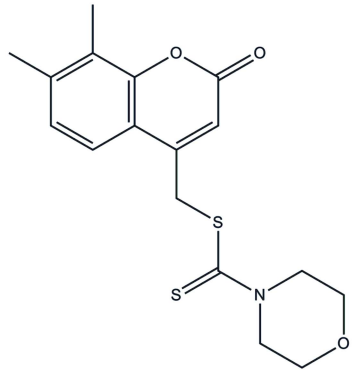
In the title compound, $C_{17}H_{19}NO_3S_2$, the chromene unit makes a dihedral angle of 88.48 (5)° with the best plane through the morpholine ring. The carbodithioate group is present in an antiperiplanar conformation with respect to the morpholine ring, as indicated by the S—C—N—C torsion angle of −171.64 (8)°. The morpholine moiety adopts the usual chair conformation. The crystal structure features C—H···O and C—H···S hydrogen bonds and C—H···π interactions.

3D view



Chemical scheme



Structure description

Coumarins and its derivatives have drawn much attention in the field of current medicinal and pharmacological research and are reported to have a broad spectrum of biological activities, such as antimicrobial (Ronad *et al.*, 2010) and anti-inflammatory (Eissa *et al.*, 2009) properties. In addition, dithiocarbamic acid esters have gained a prominent role as cancer chemopreventive and anticancer agents (Scozzafava *et al.*, 2000). In view of their importance, the crystal structure determination of the title compound was carried out and the results are presented herein.

In the molecular structure of the title compound (Fig. 1), the mean planes of the chromene unit and morpholine rings make a dihedral angle of 88.48 (5)°. The heterocyclic morpholine ring adopts a chair conformation with puckering parameters Q = 0.5323 (13) Å, θ = 10.75 (12)° and φ = 354.1 (8)°.

The two methyl groups are essentially coplanar with the chromene moiety, the maximum deviation from the mean plane being 0.040 (2) and 0.029 (2) Å for atoms C7 and C8, respectively. The carbodithioate group is present in an antiperiplanar confor-

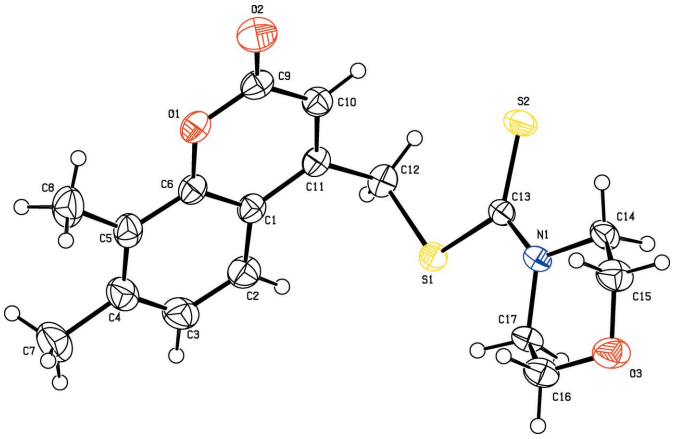


Figure 1
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50° probability level. H atoms are represented as small circles.

mation with respect to the morpholine ring, as indicated by the S2—C13—N1—C17 torsion angle of −171.64 (8)°. In the crystal, C12—H12*B*···O2 and C17—H17*A*···S2 hydrogen bonds (Table 1) result in the formation of chains along the *b* axis (Fig. 2). Parallel chains are linked by C—H···π interactions.

Synthesis and crystallization

4-Bromomethyl-6,7-dimethyl-chromen-2-one (3.9 g, 0.015 mol) and the potassium salt of morpholine-4-carboxylate (2.5 g, 0.015 mol) were dissolved in 35 ml of absolute ethanol and stirred at room temperature for 14 h. After completion of the reaction (monitored by TLC) ethanol was removed under reduced pressure. The solid obtained was extracted in ethyl acetate, washed with water, and the collected organic extract was dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the obtained solid product was crystallized from an ethanol:chloroform mixture (7:3) by slow evaporation.

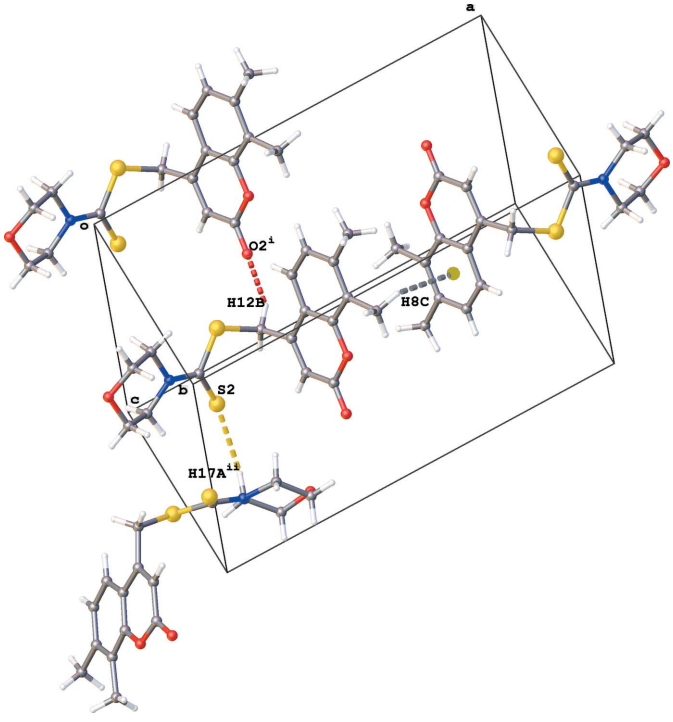


Figure 2
A crystal packing diagram of the title molecule, showing the C—H···O, C—H···S and C—H···π hydrogen bonds as red, yellow and gray dashed lines, respectively.

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

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*B*···O2^{i}	0.97	2.38	3.2731 (15)	153
C17—H17*A*···S2^{ii}	0.97	2.86	3.6412 (11)	138
C8—H8*C*···*Cg*^{iii}	0.96	2.93	3.6540 (17)	133

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

Refinement

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

Acknowledgements

The authors would like to thank the SJB Institute of Technology, Kengeri, Bangalore, for their support. MM would also

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{19}NO_3S_2$
M_r	349.47
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	16.0366 (5), 7.8085 (2), 13.5083 (4)
β (°)	93.899 (1)
V (Å^3)	1687.62 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.33
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD area-detector diffractometer
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26234, 7073, 5320
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.800
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.119, 1.02
No. of reflections	7073
No. of parameters	210
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.22

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009).

like to thank the UGC, New Delhi, Government of India, for awarding project F.41–920/2012(SR).

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full crystallographic data

IUCrData (2016). **1**, x160084 [doi:10.1107/S2414314616000845]

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(7, 8-Dimethyl-2-oxo-2*H*-chromen-4-yl)methyl morpholine-4-carbodithioate

Crystal data

$C_{17}H_{19}NO_3S_2$
M_r = 349.47
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 16.0366 (5) Å
b = 7.8085 (2) Å
c = 13.5083 (4) Å
β = 93.899 (1)°
V = 1687.62 (8) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7073 reflections
θ = 2.6–34.7°
μ = 0.33 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
ω and φ scans
26234 measured reflections
7073 independent reflections
5320 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 34.7°, θ_{min} = 2.6°
h = −25→25
k = −11→12
l = −19→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.119
S = 1.02
7073 reflections
210 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.1849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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 on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.13237 (2)	0.68580 (3)	0.11577 (2)	0.0365 (1)
S2	0.06981 (2)	0.86839 (4)	0.29369 (2)	0.0437 (1)
O1	0.34619 (5)	1.17857 (10)	0.08292 (7)	0.0410 (3)
O2	0.29328 (8)	1.33313 (12)	0.19925 (9)	0.0590 (4)
O3	−0.17623 (6)	0.83041 (14)	0.01555 (8)	0.0548 (3)
N1	−0.02040 (5)	0.79973 (11)	0.12636 (6)	0.0316 (2)
C1	0.31549 (6)	0.87734 (13)	0.06476 (9)	0.0350 (3)
C2	0.32454 (8)	0.72858 (16)	0.00852 (11)	0.0456 (3)
C3	0.36730 (9)	0.7350 (2)	−0.07620 (11)	0.0531 (4)
C4	0.40227 (8)	0.8863 (2)	−0.10921 (10)	0.0502 (4)
C5	0.39485 (7)	1.03644 (17)	−0.05460 (10)	0.0438 (3)
C6	0.35172 (6)	1.02710 (14)	0.03136 (9)	0.0363 (3)
C7	0.44803 (10)	0.8850 (3)	−0.20342 (13)	0.0700 (6)
C8	0.43010 (10)	1.2049 (2)	−0.08649 (13)	0.0612 (5)
C9	0.30067 (7)	1.19183 (14)	0.16390 (10)	0.0405 (3)
C10	0.26574 (7)	1.03691 (14)	0.20165 (9)	0.0382 (3)
C11	0.27068 (6)	0.88575 (13)	0.15391 (8)	0.0336 (3)
C12	0.22768 (7)	0.73014 (14)	0.19169 (9)	0.0381 (3)
C13	0.05326 (6)	0.79190 (11)	0.17926 (7)	0.0298 (2)
C14	−0.09634 (7)	0.85250 (16)	0.17357 (9)	0.0395 (3)
C15	−0.15855 (8)	0.93490 (18)	0.10023 (10)	0.0497 (4)
C16	−0.10252 (8)	0.80537 (17)	−0.03374 (9)	0.0450 (3)
C17	−0.03728 (7)	0.71207 (14)	0.03087 (8)	0.0363 (3)
H2	0.30170	0.62580	0.02850	0.0550*
H3	0.37310	0.63520	−0.11270	0.0640*
H7A	0.44790	0.77100	−0.23010	0.1050*
H7B	0.50460	0.92200	−0.18900	0.1050*
H7C	0.42060	0.96110	−0.25100	0.1050*
H8A	0.42710	1.28700	−0.03400	0.0920*
H8B	0.39830	1.24550	−0.14460	0.0920*
H8C	0.48730	1.18960	−0.10130	0.0920*
H10	0.23900	1.04120	0.26060	0.0460*
H12A	0.21440	0.74900	0.25980	0.0460*
H12B	0.26480	0.63220	0.19040	0.0460*
H14A	−0.08140	0.93270	0.22670	0.0470*
H14B	−0.12160	0.75310	0.20240	0.0470*
H15A	−0.20990	0.95680	0.13200	0.0600*
H15B	−0.13670	1.04400	0.07950	0.0600*
H16A	−0.08060	0.91560	−0.05250	0.0540*
H16B	−0.11540	0.74000	−0.09390	0.0540*
H17A	−0.05630	0.59640	0.04260	0.0440*
H17B	0.01400	0.70480	−0.00310	0.0440*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0347 (1)	0.0342 (1)	0.0411 (2)	−0.0005 (1)	0.0070 (1)	−0.0070 (1)
S2	0.0485 (2)	0.0528 (2)	0.0299 (1)	0.0005 (1)	0.0020 (1)	−0.0091 (1)
O1	0.0395 (4)	0.0336 (4)	0.0495 (5)	−0.0047 (3)	0.0010 (3)	0.0009 (3)
O2	0.0732 (7)	0.0337 (4)	0.0704 (7)	−0.0013 (4)	0.0069 (5)	−0.0122 (4)
O3	0.0412 (4)	0.0720 (7)	0.0500 (6)	0.0100 (4)	−0.0062 (4)	−0.0159 (5)
N1	0.0360 (4)	0.0323 (4)	0.0269 (4)	0.0031 (3)	0.0048 (3)	−0.0032 (3)
C1	0.0303 (4)	0.0334 (5)	0.0412 (6)	0.0018 (3)	0.0014 (4)	−0.0015 (4)
C2	0.0428 (6)	0.0389 (5)	0.0552 (7)	0.0025 (4)	0.0047 (5)	−0.0087 (5)
C3	0.0484 (7)	0.0572 (8)	0.0538 (8)	0.0086 (6)	0.0047 (5)	−0.0162 (6)
C4	0.0358 (5)	0.0723 (9)	0.0427 (7)	0.0094 (5)	0.0032 (5)	−0.0031 (6)
C5	0.0313 (5)	0.0565 (7)	0.0432 (6)	0.0008 (5)	0.0007 (4)	0.0073 (5)
C6	0.0288 (4)	0.0378 (5)	0.0418 (6)	0.0006 (4)	−0.0012 (4)	0.0006 (4)
C7	0.0518 (8)	0.1087 (14)	0.0507 (9)	0.0115 (9)	0.0131 (6)	−0.0033 (9)
C8	0.0550 (8)	0.0716 (9)	0.0576 (9)	−0.0107 (7)	0.0078 (6)	0.0177 (7)
C9	0.0394 (5)	0.0335 (5)	0.0476 (6)	0.0002 (4)	−0.0034 (5)	−0.0042 (4)
C10	0.0386 (5)	0.0353 (5)	0.0407 (6)	0.0016 (4)	0.0027 (4)	−0.0020 (4)
C11	0.0293 (4)	0.0310 (4)	0.0401 (5)	0.0021 (3)	−0.0005 (4)	0.0021 (4)
C12	0.0363 (5)	0.0329 (5)	0.0448 (6)	0.0015 (4)	0.0007 (4)	0.0066 (4)
C13	0.0372 (4)	0.0245 (4)	0.0281 (4)	−0.0008 (3)	0.0060 (3)	0.0004 (3)
C14	0.0385 (5)	0.0466 (6)	0.0344 (5)	0.0057 (4)	0.0092 (4)	−0.0051 (4)
C15	0.0458 (6)	0.0536 (7)	0.0493 (7)	0.0148 (5)	0.0005 (5)	−0.0106 (6)
C16	0.0518 (6)	0.0493 (6)	0.0331 (6)	0.0062 (5)	−0.0021 (5)	0.0000 (4)
C17	0.0436 (5)	0.0372 (5)	0.0281 (5)	0.0049 (4)	0.0030 (4)	−0.0057 (4)

Geometric parameters (Å, º)

S1—C12	1.8152 (12)	C11—C12	1.5034 (15)
S1—C13	1.7830 (10)	C14—C15	1.5021 (18)
S2—C13	1.6616 (10)	C16—C17	1.5043 (17)
O1—C6	1.3785 (14)	C2—H2	0.9300
O1—C9	1.3597 (16)	C3—H3	0.9300
O2—C9	1.2113 (15)	C7—H7A	0.9600
O3—C15	1.4179 (17)	C7—H7B	0.9600
O3—C16	1.4092 (16)	C7—H7C	0.9600
N1—C13	1.3398 (13)	C8—H8A	0.9600
N1—C14	1.4715 (14)	C8—H8B	0.9600
N1—C17	1.4691 (14)	C8—H8C	0.9600
C1—C2	1.4009 (17)	C10—H10	0.9300
C1—C6	1.3944 (15)	C12—H12A	0.9700
C1—C11	1.4452 (15)	C12—H12B	0.9700
C2—C3	1.375 (2)	C14—H14A	0.9700
C3—C4	1.394 (2)	C14—H14B	0.9700
C4—C5	1.395 (2)	C15—H15A	0.9700
C4—C7	1.512 (2)	C15—H15B	0.9700
C5—C6	1.3933 (17)	C16—H16A	0.9700

C5—C8	1.506 (2)	C16—H16B	0.9700
C9—C10	1.4408 (16)	C17—H17A	0.9700
C10—C11	1.3499 (15)	C17—H17B	0.9700
S1···C2	3.5093 (14)	C8···H7C	2.9200
S2···C17^{i}	3.6412 (11)	C8···H7B	2.9100
S2···C10	3.6988 (12)	C9···H8B^{vii}	2.9700
S1···H2	3.0700	C12···H2	2.7000
S1···H17B	2.4100	C13···H16A^{iv}	2.9100
S1···H14A^{ii}	3.0600	C13···H14A^{ii}	3.1000
S1···H17A	3.2000	C17···H17A^{ix}	3.0400
S2···H12A	2.5700	H2···S1	3.0700
S2···H14A	2.5800	H2···C12	2.7000
S2···H10	3.0900	H2···H12B	2.3000
S2···H14B^{i}	3.1200	H3···H7A	2.3100
S2···H17A^{i}	2.8600	H7A···H3	2.3100
S2···H17B^{iii}	3.0000	H7B···C8	2.9100
O1···O3^{iv}	2.9513 (13)	H7B···H8C	2.4300
O2···C12^{v}	3.2731 (15)	H7B···O1^{vi}	2.8200
O3···O1^{iv}	2.9513 (13)	H7B···C6^{vi}	3.0600
O3···C10^{iv}	3.3421 (16)	H7C···C8	2.9200
O3···C6^{iv}	3.0524 (14)	H7C···O2^{x}	2.6500
O3···C9^{iv}	3.0382 (16)	H8A···O1	2.2700
O3···C1^{iv}	3.3230 (15)	H8B···C7	3.0500
O3···N1	2.8345 (13)	H8B···O2^{x}	2.6800
O1···H8A	2.2700	H8B···C9^{x}	2.9700
O1···H7B^{vi}	2.8200	H8C···C7	2.8000
O2···H8B^{vii}	2.6800	H8C···H7B	2.4300
O2···H12B^{v}	2.3800	H10···S2	3.0900
O2···H15A^{i}	2.8900	H10···H12A	2.3200
O2···H7C^{vii}	2.6500	H10···H14B^{i}	2.5800
N1···O3	2.8345 (13)	H12A···S2	2.5700
C1···O3^{iv}	3.3230 (15)	H12A···H10	2.3200
C1···C15^{iv}	3.5620 (17)	H12B···O2^{viii}	2.3800
C2···S1	3.5093 (14)	H12B···C2	2.8000
C6···C15^{iv}	3.4778 (17)	H12B···H2	2.3000
C6···O3^{iv}	3.0524 (14)	H14A···S2	2.5800
C9···C16^{iv}	3.5256 (17)	H14A···S1^{i}	3.0600
C9···O3^{iv}	3.0382 (16)	H14A···C13^{i}	3.1000
C10···C16^{iv}	3.5644 (17)	H14B···S2^{ii}	3.1200
C10···S2	3.6988 (12)	H14B···H10^{ii}	2.5800
C10···O3^{iv}	3.3421 (16)	H15A···O2^{ii}	2.8900
C12···O2^{viii}	3.2731 (15)	H15A···C5^{iv}	3.0800
C15···C1^{iv}	3.5620 (17)	H15A···C6^{iv}	3.0600
C15···C6^{iv}	3.4778 (17)	H15B···H16A	2.2800
C16···C10^{iv}	3.5644 (17)	H16A···H15B	2.2800
C16···C9^{iv}	3.5256 (17)	H16A···C13^{iv}	2.9100
C17···S2^{ii}	3.6412 (11)	H17A···S1	3.2000

C2···H12B	2.8000	H17A···S2^{ii}	2.8600
C5···H15A^{iv}	3.0800	H17A···C17^{ix}	3.0400
C6···H7B^{vi}	3.0600	H17A···H17B^{ix}	2.5200
C6···H15A^{iv}	3.0600	H17B···S1	2.4100
C7···H8B	3.0500	H17B···H17A^{ix}	2.5200
C7···H8C	2.8000	H17B···S2^{xi}	3.0000

C12—S1—C13	103.82 (5)	C4—C7—H7A	109.00
C6—O1—C9	121.89 (9)	C4—C7—H7B	109.00
C15—O3—C16	109.44 (10)	C4—C7—H7C	109.00
C13—N1—C14	120.48 (8)	H7A—C7—H7B	109.00
C13—N1—C17	123.38 (8)	H7A—C7—H7C	109.00
C14—N1—C17	113.73 (8)	H7B—C7—H7C	109.00
C2—C1—C6	117.33 (11)	C5—C8—H8A	109.00
C2—C1—C11	124.42 (10)	C5—C8—H8B	109.00
C6—C1—C11	118.25 (10)	C5—C8—H8C	109.00
C1—C2—C3	119.82 (12)	H8A—C8—H8B	109.00
C2—C3—C4	122.11 (14)	H8A—C8—H8C	110.00
C3—C4—C5	119.51 (12)	H8B—C8—H8C	109.00
C3—C4—C7	119.51 (15)	C9—C10—H10	119.00
C5—C4—C7	120.98 (14)	C11—C10—H10	119.00
C4—C5—C6	117.51 (12)	S1—C12—H12A	110.00
C4—C5—C8	122.39 (12)	S1—C12—H12B	109.00
C6—C5—C8	120.09 (12)	C11—C12—H12A	110.00
O1—C6—C1	120.90 (10)	C11—C12—H12B	110.00
O1—C6—C5	115.39 (10)	H12A—C12—H12B	108.00
C1—C6—C5	123.71 (11)	N1—C14—H14A	109.00
O1—C9—O2	117.31 (11)	N1—C14—H14B	109.00
O1—C9—C10	117.63 (10)	C15—C14—H14A	109.00
O2—C9—C10	125.06 (12)	C15—C14—H14B	109.00
C9—C10—C11	121.88 (11)	H14A—C14—H14B	108.00
C1—C11—C10	119.11 (10)	O3—C15—H15A	109.00
C1—C11—C12	120.78 (9)	O3—C15—H15B	109.00
C10—C11—C12	120.09 (10)	C14—C15—H15A	109.00
S1—C12—C11	110.51 (8)	C14—C15—H15B	109.00
S1—C13—S2	122.73 (6)	H15A—C15—H15B	108.00
S1—C13—N1	113.27 (7)	O3—C16—H16A	109.00
S2—C13—N1	123.99 (7)	O3—C16—H16B	109.00
N1—C14—C15	111.48 (10)	C17—C16—H16A	109.00
O3—C15—C14	111.90 (11)	C17—C16—H16B	109.00
O3—C16—C17	111.45 (10)	H16A—C16—H16B	108.00
N1—C17—C16	111.29 (9)	N1—C17—H17A	109.00
C1—C2—H2	120.00	N1—C17—H17B	109.00
C3—C2—H2	120.00	C16—C17—H17A	109.00
C2—C3—H3	119.00	C16—C17—H17B	109.00
C4—C3—H3	119.00	H17A—C17—H17B	108.00

C13—S1—C12—C11	−93.89 (8)	C2—C1—C11—C10	−179.63 (11)

C12—S1—C13—S2	−12.19 (7)	C2—C1—C11—C12	−1.54 (17)
C12—S1—C13—N1	169.21 (7)	C6—C1—C11—C10	−0.26 (15)
C9—O1—C6—C1	−4.71 (16)	C6—C1—C11—C12	177.83 (10)
C9—O1—C6—C5	174.95 (10)	C1—C2—C3—C4	−0.3 (2)
C6—O1—C9—O2	−173.62 (11)	C2—C3—C4—C5	0.7 (2)
C6—O1—C9—C10	7.02 (16)	C2—C3—C4—C7	−179.57 (14)
C16—O3—C15—C14	−61.85 (14)	C3—C4—C5—C6	−0.31 (18)
C15—O3—C16—C17	62.58 (13)	C3—C4—C5—C8	−179.20 (13)
C14—N1—C13—S1	168.24 (8)	C7—C4—C5—C6	179.98 (11)
C14—N1—C13—S2	−10.34 (13)	C7—C4—C5—C8	1.1 (2)
C17—N1—C13—S1	6.94 (12)	C4—C5—C6—O1	179.86 (10)
C17—N1—C13—S2	−171.64 (8)	C4—C5—C6—C1	−0.50 (17)
C13—N1—C14—C15	151.92 (10)	C8—C5—C6—O1	−1.22 (16)
C17—N1—C14—C15	−45.09 (13)	C8—C5—C6—C1	178.42 (12)
C13—N1—C17—C16	−151.69 (10)	O1—C9—C10—C11	−6.16 (17)
C14—N1—C17—C16	45.88 (12)	O2—C9—C10—C11	174.54 (13)
C6—C1—C2—C3	−0.47 (18)	C9—C10—C11—C1	2.81 (16)
C11—C1—C2—C3	178.91 (12)	C9—C10—C11—C12	−175.29 (10)
C2—C1—C6—O1	−179.49 (10)	C1—C11—C12—S1	−74.77 (11)
C2—C1—C6—C5	0.89 (17)	C10—C11—C12—S1	103.30 (11)
C11—C1—C6—O1	1.10 (15)	N1—C14—C15—O3	52.85 (14)
C11—C1—C6—C5	−178.53 (10)	O3—C16—C17—N1	−54.64 (13)

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*, −*y*+2, −*z*; (v) *x*, *y*+1, *z*; (vi) −*x*+1, −*y*+2, −*z*; (vii) *x*, −*y*+5/2, *z*+1/2; (viii) *x*, *y*−1, *z*; (ix) −*x*, −*y*+1, −*z*; (x) *x*, −*y*+5/2, *z*−1/2; (xi) *x*, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*B*···O2^{viii}	0.97	2.38	3.2731 (15)	153
C17—H17*A*···S2^{ii}	0.97	2.86	3.6412 (11)	138
C8—H8*C*···*Cg*^{vi}	0.96	2.93	3.6540 (17)	133

Symmetry codes: (ii) −*x*, *y*−1/2, −*z*+1/2; (vi) −*x*+1, −*y*+2, −*z*; (viii) *x*, *y*−1, *z*.