

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(Z)-3-(2-Methoxybenzyl)-1,5-benzothiazepin-4(5H)-oneR. Selvakumar,^a M. Bakthadoss,^{a‡} D. Lakshmanan^b and S. Murugavel^{c*}

^aDepartment of Organic Chemistry, University of Madras, Maraimalai Campus, Chennai 600 025, India, ^bDepartment of Physics, C. Abdul Hakeem College of Engineering & Technology, Melvisharam, Vellore 632 509, India, and ^cDepartment of Physics, Thanthai Periyar Government Institute of Technology, Vellore 632 002, India

Correspondence e-mail: smurugavel27@gmail.com

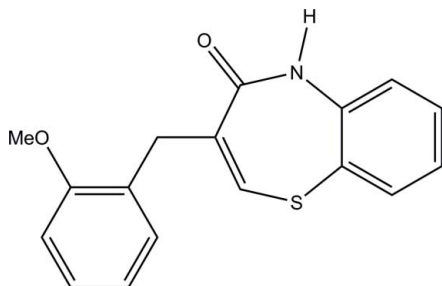
Received 10 June 2012; accepted 12 June 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.046; wR factor = 0.146; data-to-parameter ratio = 21.7.

In the title compound, $\text{C}_{17}\text{H}_{15}\text{NO}_2\text{S}$, the seven-membered thiazepine ring adopts a distorted twist-boat conformation. The dihedral angle between the mean planes of the benzothiazepin ring system and the attached benzene ring is 47.7 (1)°. In the crystal, pairs of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link inversion-related molecules into dimers, generating $R_2^2(8)$ ring motifs. These dimers are further connected into a chain along the a axis by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in $R_2^2(14)$ ring motifs. The crystal packing also features $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For the pharmaceutical properties of thiazepin derivatives, see: Tomascovic *et al.* (2000). For related structures, see: Sridevi *et al.* (2011); Sabari *et al.* (2011). For ring-puckering parameters, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{17}\text{H}_{15}\text{NO}_2\text{S}$ $M_r = 297.36$

Triclinic, $P\bar{1}$
 $a = 8.6665$ (5) Å
 $b = 9.7612$ (4) Å
 $c = 10.1328$ (5) Å
 $\alpha = 108.181$ (3)°
 $\beta = 101.561$ (2)°
 $\gamma = 103.217$ (3)°

$V = 757.83$ (7) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.22$ mm⁻¹
 $T = 293$ K
 $0.23 \times 0.21 \times 0.15$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.951$, $T_{\max} = 0.968$

16048 measured reflections
 4137 independent reflections
 2797 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.146$
 $S = 1.01$
 4137 reflections

191 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C11–C16 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.86	2.00	2.8545 (17)	171
$\text{C5}-\text{H5}\cdots\text{O1}^{\text{ii}}$	0.93	2.39	3.308 (2)	171
$\text{C3}-\text{H3}\cdots\text{Cg}^{\text{iii}}$	0.93	2.69	3.432 (2)	138
$\text{C17}-\text{H17C}\cdots\text{Cg}^{\text{iv}}$	0.96	2.90	3.664 (2)	137

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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)); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

The authors thank Dr Babu Vargheese, SAIF, IIT, Madras, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6847).

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supporting information

Acta Cryst. (2012). E68, o2126 [https://doi.org/10.1107/S160053681202661X]

(Z)-3-(2-Methoxybenzyl)-1,5-benzothiazepin-4(5H)-one**R. Selvakumar, M. Bakthadoss, D. Lakshmanan and S. Murugavel****S1. Comment**

The title compound is used as an intermediate for the synthesis of dosulepin, which is an antidepressant of the tricyclic family. Dosulepin prevents reabsorbing of serotonin and noradrenaline in the brain, helps to prolong the mood lightening effect of any released noradrenaline and serotonin, thus relieving depression. The dibenzo[c,e]thiazepin derivatives exhibit chiroptical properties (Tomascovic *et al.*, 2000). As part of our studies in this area, we now describe the crystal structure of the title compound, (I).

Fig. 1. shows a displacement ellipsoid plot of (I), with the atom numbering scheme. The seven membered thiazepine ring (N1/S1/C1/C2/C7/C8/C9) adopts twist-boat conformation as indicated by puckering parameters (Cremer & Pople, 1975) $QT = 1.0218(14) \text{ \AA}$, $\theta_2 = 74.4(1)^\circ$, $\varphi_2 = 178.1(1)^\circ$ and $\varphi_3 = 174.3(4)^\circ$. The dihedral angle between the benzothiazepin ring system and the benzene ring is $47.7(1)^\circ$. The geometric parameters of the title molecule agree well with those reported for similar structures (Sridevi *et al.*, 2011, Sabari *et al.*, 2011).

In the crystal, the molecules at x, y, z and $-x, 1-y, -z$ are linked by N1—H1 \cdots O1 hydrogen bonds into cyclic centrosymmetric $R_2^2(8)$ dimers (Bernstein *et al.*, 1995). These dimers are further connected into chains along the a axis via C5—H5 \cdots O1 hydrogen bonds (Table 1), resulting in $R_2^2(14)$ ring motifs [Fig. 2; symmetry code as in Fig. 2].

The crystal packing also features two C—H \cdots π interactions, the first one between a H3 atom and neighbouring benzene ring (C11—C16), with a C3—H3 \cdots Cgⁱⁱⁱ separation of 2.69 \AA and the second one between methyl H17C atom and neighbouring benzene ring (C11—C16), with a C17—H17C \cdots Cg^{iv} separation of 2.90 \AA (Fig. 3 and Table 1; Cg is the centroid of the C11—C16 benzene ring, Symmetry code as in Fig.3).

S2. Experimental

A mixture of (*Z*)-methyl 2-(bromomethyl)-3-(2-methoxyphenyl)acrylate (2 mmol) and *o*-aminothiophenol (2 mmol) in the presence of potassium *tert*-butoxide (4.8 mmol) in dry THF (10 ml) was stirred at room temperature for 1 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (20 ml) and extracted with ethyl acetate (3 x 20 ml). The organic layer was washed with brine (2 x 20 ml) and dried over anhydrous sodium sulfate. The organic layer was concentrated, which successfully provide the crude final product ((*Z*)-3-(2-methoxybenzyl)benzo[*b*][1,4]thiazepin-4(5H)-one). The final product was purified by column chromatography on silica gel to afford the title compound in good yield (42%). Recrystallisation from ethyl acetate solution afforded colourless blocks.

S3. Refinement

H atoms were positioned geometrically, with C—H = $0.93\text{--}0.97 \text{ \AA}$ and constrained to ride on their parent atom, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

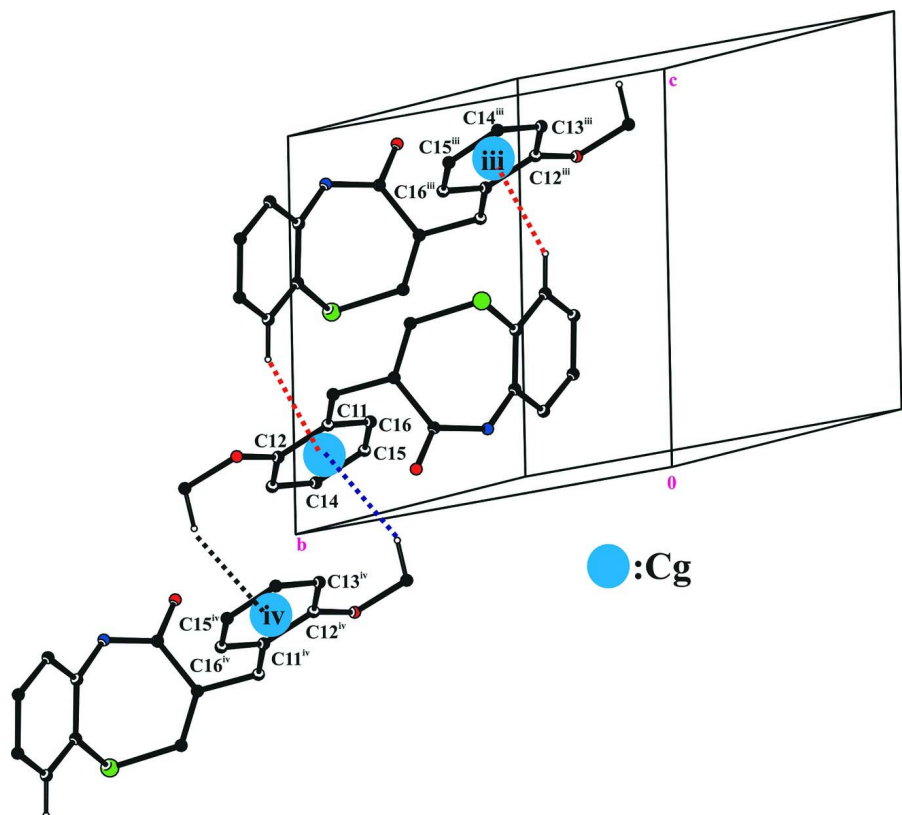


Figure 3

A view of the C—H... π interactions, in the crystal structure of the title compound. Cg is the centroid of the (C11–C16) benzene ring. [Symmetry code: (iii) $1 - x, 2 - y, 1 - z$; (iv) $-x, 2 - y, -z$.]

(Z)-3-(2-Methoxybenzyl)-1,5-benzothiazepin-4(5H)-one

Crystal data

$C_{17}H_{15}NO_2S$

$M_r = 297.36$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.6665$ (5) Å

$b = 9.7612$ (4) Å

$c = 10.1328$ (5) Å

$\alpha = 108.181$ (3)°

$\beta = 101.561$ (2)°

$\gamma = 103.217$ (3)°

$V = 757.83$ (7) Å³

$Z = 2$

$F(000) = 312$

$D_x = 1.303$ Mg m⁻³

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

Cell parameters from 4197 reflections

$\theta = 2.2$ – 29.5 °

$\mu = 0.22$ mm⁻¹

$T = 293$ K

Block, colourless

$0.23 \times 0.21 \times 0.15$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.0 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.951$, $T_{\max} = 0.968$

16048 measured reflections

4137 independent reflections

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

$R_{\text{int}} = 0.041$

$\theta_{\max} = 29.5^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -10 \rightarrow 11$

$k = -13 \rightarrow 13$
 $l = -13 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.146$
 $S = 1.01$
 4137 reflections
 191 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
 $w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.1349P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

Special details

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1759 (2)	0.7930 (2)	0.46956 (18)	0.0507 (4)
H1A	0.1877	0.8740	0.5533	0.061*
C2	0.3850 (2)	0.64173 (18)	0.39653 (19)	0.0488 (4)
C3	0.5478 (2)	0.6617 (2)	0.4686 (2)	0.0608 (5)
H3	0.5776	0.6775	0.5668	0.073*
C4	0.6642 (2)	0.6582 (2)	0.3954 (3)	0.0722 (6)
H4	0.7726	0.6702	0.4437	0.087*
C5	0.6218 (2)	0.6371 (3)	0.2510 (3)	0.0750 (7)
H5	0.7016	0.6348	0.2018	0.090*
C6	0.4611 (2)	0.6192 (2)	0.1781 (2)	0.0599 (5)
H6	0.4332	0.6057	0.0803	0.072*
C7	0.34186 (19)	0.62133 (17)	0.25091 (18)	0.0451 (4)
C8	0.07211 (19)	0.67234 (17)	0.20182 (16)	0.0411 (3)
C9	0.11639 (19)	0.80262 (17)	0.34308 (17)	0.0424 (4)
C10	0.0753 (2)	0.93974 (18)	0.33034 (18)	0.0486 (4)
H10A	0.0944	1.0126	0.4271	0.058*
H10B	-0.0416	0.9100	0.2793	0.058*
C11	0.1745 (2)	1.01587 (18)	0.25198 (17)	0.0470 (4)
C12	0.1171 (2)	1.11473 (19)	0.19637 (17)	0.0513 (4)
C13	0.2044 (3)	1.1847 (2)	0.1219 (2)	0.0668 (5)
H13	0.1647	1.2489	0.0831	0.080*
C14	0.3502 (3)	1.1584 (3)	0.1058 (2)	0.0756 (6)
H14	0.4084	1.2051	0.0556	0.091*

C15	0.4107 (3)	1.0648 (3)	0.1623 (2)	0.0704 (6)
H15	0.5102	1.0490	0.1521	0.085*
C16	0.3221 (2)	0.9936 (2)	0.2350 (2)	0.0568 (5)
H16	0.3629	0.9294	0.2732	0.068*
C17	-0.0912 (3)	1.2357 (2)	0.1686 (2)	0.0704 (6)
H17A	-0.0129	1.3361	0.2124	0.106*
H17B	-0.1929	1.2378	0.1917	0.106*
H17C	-0.1121	1.2002	0.0650	0.106*
N1	0.17774 (16)	0.59507 (15)	0.17075 (14)	0.0454 (3)
H1	0.1400	0.5180	0.0899	0.055*
O1	-0.06363 (14)	0.63859 (14)	0.11211 (12)	0.0530 (3)
O2	-0.02545 (17)	1.13659 (15)	0.22258 (14)	0.0595 (3)
S1	0.23445 (6)	0.63866 (6)	0.49135 (5)	0.05956 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0560 (10)	0.0537 (9)	0.0413 (8)	0.0174 (8)	0.0217 (7)	0.0116 (7)
C2	0.0453 (9)	0.0419 (8)	0.0522 (9)	0.0133 (7)	0.0104 (7)	0.0113 (7)
C3	0.0508 (10)	0.0505 (10)	0.0644 (11)	0.0137 (8)	0.0004 (9)	0.0117 (8)
C4	0.0417 (10)	0.0606 (12)	0.0915 (16)	0.0142 (9)	0.0038 (10)	0.0098 (11)
C5	0.0451 (11)	0.0719 (13)	0.1002 (18)	0.0195 (9)	0.0327 (11)	0.0139 (12)
C6	0.0474 (10)	0.0650 (11)	0.0615 (11)	0.0185 (8)	0.0232 (8)	0.0108 (9)
C7	0.0377 (8)	0.0405 (8)	0.0489 (9)	0.0114 (6)	0.0122 (7)	0.0070 (6)
C8	0.0380 (8)	0.0453 (8)	0.0398 (7)	0.0105 (6)	0.0167 (6)	0.0141 (6)
C9	0.0404 (8)	0.0444 (8)	0.0435 (8)	0.0125 (6)	0.0207 (7)	0.0130 (6)
C10	0.0539 (10)	0.0462 (8)	0.0507 (9)	0.0177 (7)	0.0272 (8)	0.0158 (7)
C11	0.0503 (9)	0.0412 (8)	0.0405 (8)	0.0065 (7)	0.0170 (7)	0.0069 (6)
C12	0.0579 (10)	0.0475 (9)	0.0393 (8)	0.0071 (8)	0.0151 (7)	0.0103 (7)
C13	0.0782 (14)	0.0627 (12)	0.0582 (11)	0.0106 (10)	0.0229 (10)	0.0274 (9)
C14	0.0785 (15)	0.0759 (14)	0.0739 (14)	0.0068 (11)	0.0413 (12)	0.0306 (11)
C15	0.0611 (12)	0.0689 (13)	0.0770 (14)	0.0082 (10)	0.0382 (11)	0.0193 (11)
C16	0.0556 (10)	0.0518 (9)	0.0580 (10)	0.0113 (8)	0.0238 (9)	0.0134 (8)
C17	0.0779 (14)	0.0669 (12)	0.0699 (13)	0.0253 (11)	0.0168 (11)	0.0314 (10)
N1	0.0398 (7)	0.0468 (7)	0.0403 (7)	0.0128 (6)	0.0114 (5)	0.0047 (5)
O1	0.0427 (6)	0.0618 (7)	0.0467 (6)	0.0197 (5)	0.0108 (5)	0.0092 (5)
O2	0.0643 (8)	0.0612 (8)	0.0620 (8)	0.0232 (6)	0.0230 (6)	0.0295 (6)
S1	0.0660 (3)	0.0692 (3)	0.0533 (3)	0.0255 (2)	0.0227 (2)	0.0295 (2)

Geometric parameters (Å, °)

C1—C9	1.323 (2)	C10—C11	1.507 (2)
C1—S1	1.7571 (19)	C10—H10A	0.9700
C1—H1A	0.9300	C10—H10B	0.9700
C2—C7	1.385 (2)	C11—C16	1.381 (3)
C2—C3	1.391 (3)	C11—C12	1.394 (3)
C2—S1	1.7687 (18)	C12—O2	1.364 (2)
C3—C4	1.367 (3)	C12—C13	1.386 (3)

C3—H3	0.9300	C13—C14	1.376 (3)
C4—C5	1.371 (3)	C13—H13	0.9300
C4—H4	0.9300	C14—C15	1.365 (4)
C5—C6	1.382 (3)	C14—H14	0.9300
C5—H5	0.9300	C15—C16	1.385 (3)
C6—C7	1.386 (2)	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300
C7—N1	1.410 (2)	C17—O2	1.421 (2)
C8—O1	1.2353 (19)	C17—H17A	0.9600
C8—N1	1.338 (2)	C17—H17B	0.9600
C8—C9	1.495 (2)	C17—H17C	0.9600
C9—C10	1.497 (2)	N1—H1	0.8600
C9—C1—S1	124.92 (13)	C11—C10—H10B	108.8
C9—C1—H1A	117.5	H10A—C10—H10B	107.7
S1—C1—H1A	117.5	C16—C11—C12	118.41 (16)
C7—C2—C3	119.73 (17)	C16—C11—C10	122.51 (17)
C7—C2—S1	120.79 (13)	C12—C11—C10	119.07 (15)
C3—C2—S1	119.47 (15)	O2—C12—C13	124.34 (18)
C4—C3—C2	120.2 (2)	O2—C12—C11	115.28 (15)
C4—C3—H3	119.9	C13—C12—C11	120.37 (18)
C2—C3—H3	119.9	C14—C13—C12	119.5 (2)
C3—C4—C5	120.27 (18)	C14—C13—H13	120.2
C3—C4—H4	119.9	C12—C13—H13	120.2
C5—C4—H4	119.9	C15—C14—C13	121.1 (2)
C4—C5—C6	120.4 (2)	C15—C14—H14	119.4
C4—C5—H5	119.8	C13—C14—H14	119.4
C6—C5—H5	119.8	C14—C15—C16	119.2 (2)
C5—C6—C7	119.9 (2)	C14—C15—H15	120.4
C5—C6—H6	120.1	C16—C15—H15	120.4
C7—C6—H6	120.1	C11—C16—C15	121.4 (2)
C2—C7—C6	119.57 (16)	C11—C16—H16	119.3
C2—C7—N1	122.33 (15)	C15—C16—H16	119.3
C6—C7—N1	118.03 (15)	O2—C17—H17A	109.5
O1—C8—N1	120.15 (13)	O2—C17—H17B	109.5
O1—C8—C9	118.65 (14)	H17A—C17—H17B	109.5
N1—C8—C9	121.18 (14)	O2—C17—H17C	109.5
C1—C9—C8	122.35 (15)	H17A—C17—H17C	109.5
C1—C9—C10	122.86 (14)	H17B—C17—H17C	109.5
C8—C9—C10	114.62 (14)	C8—N1—C7	129.58 (13)
C9—C10—C11	113.97 (14)	C8—N1—H1	115.2
C9—C10—H10A	108.8	C7—N1—H1	115.2
C11—C10—H10A	108.8	C12—O2—C17	118.25 (15)
C9—C10—H10B	108.8	C1—S1—C2	98.07 (8)
C7—C2—C3—C4	-1.3 (3)	C16—C11—C12—O2	-177.21 (14)
S1—C2—C3—C4	177.35 (15)	C10—C11—C12—O2	1.7 (2)
C2—C3—C4—C5	0.9 (3)	C16—C11—C12—C13	2.0 (2)

C3—C4—C5—C6	0.0 (3)	C10—C11—C12—C13	-179.04 (16)
C4—C5—C6—C7	-0.5 (3)	O2—C12—C13—C14	177.81 (17)
C3—C2—C7—C6	0.8 (3)	C11—C12—C13—C14	-1.4 (3)
S1—C2—C7—C6	-177.84 (13)	C12—C13—C14—C15	-0.2 (3)
C3—C2—C7—N1	177.65 (15)	C13—C14—C15—C16	1.0 (3)
S1—C2—C7—N1	-1.0 (2)	C12—C11—C16—C15	-1.2 (3)
C5—C6—C7—C2	0.1 (3)	C10—C11—C16—C15	179.90 (17)
C5—C6—C7—N1	-176.89 (17)	C14—C15—C16—C11	-0.3 (3)
S1—C1—C9—C8	7.8 (2)	O1—C8—N1—C7	174.44 (16)
S1—C1—C9—C10	-177.20 (12)	C9—C8—N1—C7	-4.2 (3)
O1—C8—C9—C1	131.77 (18)	C2—C7—N1—C8	50.9 (3)
N1—C8—C9—C1	-49.6 (2)	C6—C7—N1—C8	-132.22 (18)
O1—C8—C9—C10	-43.6 (2)	C13—C12—O2—C17	1.0 (3)
N1—C8—C9—C10	135.01 (16)	C11—C12—O2—C17	-179.81 (15)
C1—C9—C10—C11	118.63 (18)	C9—C1—S1—C2	58.22 (17)
C8—C9—C10—C11	-66.03 (18)	C7—C2—S1—C1	-60.82 (15)
C9—C10—C11—C16	-19.6 (2)	C3—C2—S1—C1	120.55 (15)
C9—C10—C11—C12	161.57 (14)		

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

Cg is the centroid of the C11–C16 ring.

<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>
N1—H1 \cdots O1 ⁱ	0.86	2.00	2.8545 (17)	171
C5—H5 \cdots O1 ⁱⁱ	0.93	2.39	3.308 (2)	171
C3—H3 \cdots Cg ⁱⁱⁱ	0.93	2.69	3.432 (2)	138
C17—H17C \cdots Cg ^{iv}	0.96	2.90	3.664 (2)	137

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