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6-Bromo-2-[(*E*)-thiophen-2-ylmethylidene]-2,3,4,9-tetrahydro-1*H*-carbazol-1-one

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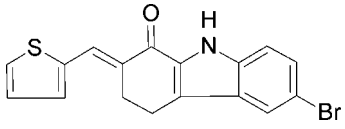
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.047; wR factor = 0.148; data-to-parameter ratio = 23.5.

In the title compound, $C_{17}H_{12}BrNOS$, the cyclohexene ring deviates only slightly from planarity (r.m.s. deviation for non-H atoms = 0.047 Å). In the crystal, the molecules are linked into centrosymmetric $R_2^2(10)$ dimers *via* pairs of N—H···O hydrogen bonds. The thiophene ring is disordered over two positions rotated by 180° and with a site-occupation factor of 0.843 (4) for the major occupied site.

Related literature

For the biological activity of carbazole derivatives, see: Magnus *et al.* (1992); Abraham (1975); Saxton (1983); Phillipson & Zenk (1980); Bergman & Pelcman (1990); Bonesi *et al.* (2004); Chakraborty *et al.* (1965); Kirtikar & Basu (1933); Chakraborty *et al.* (1973); Savini *et al.* (2004). For puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Nardelli (1983). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{12}BrNOS$
M_r = 358.25
Monoclinic, $P2_1/c$
a = 13.8655 (5) Å
b = 6.3081 (3) Å
c = 17.4583 (7) Å
β = 103.666 (2)°
V = 1483.76 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.91 mm^{-1}
T = 296 K
0.21 × 0.17 × 0.16 mm

Data collection

Bruker SMART APEX CCD detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.558, T_{max} = 0.628
12158 measured reflections
4487 independent reflections
1953 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
S = 0.85
4487 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	2.00	2.804 (4)	151

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5684).

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S1. Comment

Carbazole alkaloids obtained from naturally occurring sources have been the subject of extensive research, mainly because of their widespread applications in traditional medicine (Bergman & Pelcman, 1990; Bonesi *et al.*, 2004; Chakraborty *et al.*, 1965; Kirtikar & Basu, 1933). Tetrahydrocarbazole systems are present in the framework of a number of indole-type alkaloids of biological interest (Magnus *et al.*, 1992; Abraham, 1975; Saxton, 1983; Phillipson *et al.*, 1980). These types of compounds possess significant antibiotic, anti-carcinogenic, antiviral and anti-inflammatory properties (Chakraborty *et al.*, 1973). The thiophene derivatives possess the antimicrobial activity (Savini *et al.*, 2004). Against this background and to ascertain the molecular structure and conformation, the X-ray crystal structure determination of the title compound has been carried out.

The *ORTEP* plot of the molecule is shown in Fig. 1. The cyclohexene ring in the carbazole ring system adopts envelope conformation with the puckering parameters (Cremer & Pople, 1975) and the asymmetry parameters (Nardelli, 1983) are: q_2=0.126 (5) Å, q_3 = 0.050 (4) Å, φ_2 = 102.0 (2)° and Δ_s(C10 & C13)= 4.4 (5)°. Thiophene ring in the molecule is planar conformation. The sum of the bond angles around N1 [359.3°] is in accordance with sp^2 hybridization.

The molecules at (*x*, *y*, *z*) and (-*x* + 2, -*y* + 1, -*z*) are linked by N1—H1···O1 hydrogen bonds into a cyclic centrosymmetric $R_2^2(14)$ dimer.

S2. Experimental

The mixed aldol condensation reaction of 6-bromo-1-oxo-1,2,3, 4-tetrahydrocarbazole reacted with thiophene-2-carbaldehyde in the presence of alcoholic KOH, afforded a single product, substituted 6-bromo-2- thiofuran-2-ylmethyl-ene-2,3,4,9-tetrahydro-carbazol-1-one. This was purified by using column chromatography over silica gel (mesh 60–80). During elution of the column with petroleum ether (60–80°C) and ethyl acetate [1:2] mixture, a yellowish solid was obtained. The crystals of the title compound suitable for single XRD analysis were obtained by the slow evaporation method using the solvent mixture ethyl acetate and acetone (8:2) at room temperature.

S3. Refinement

N-bound H atom was located in a difference map and refined isotropically. C-bound H atoms were positioned geometrically (C–H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for all other H atoms. The thiophene ring is disordered over two positions rotated by 180 degrees and with a site occupation factor of 0.843 (4) for the major occupied site.

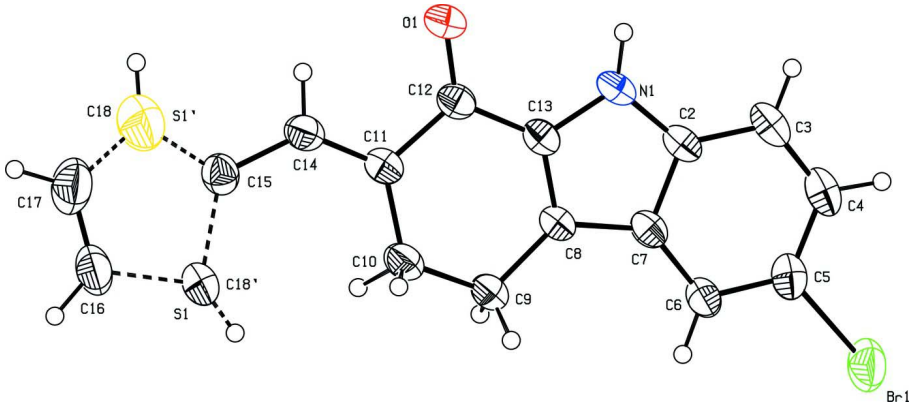

Figure 1

The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 50% probability level.

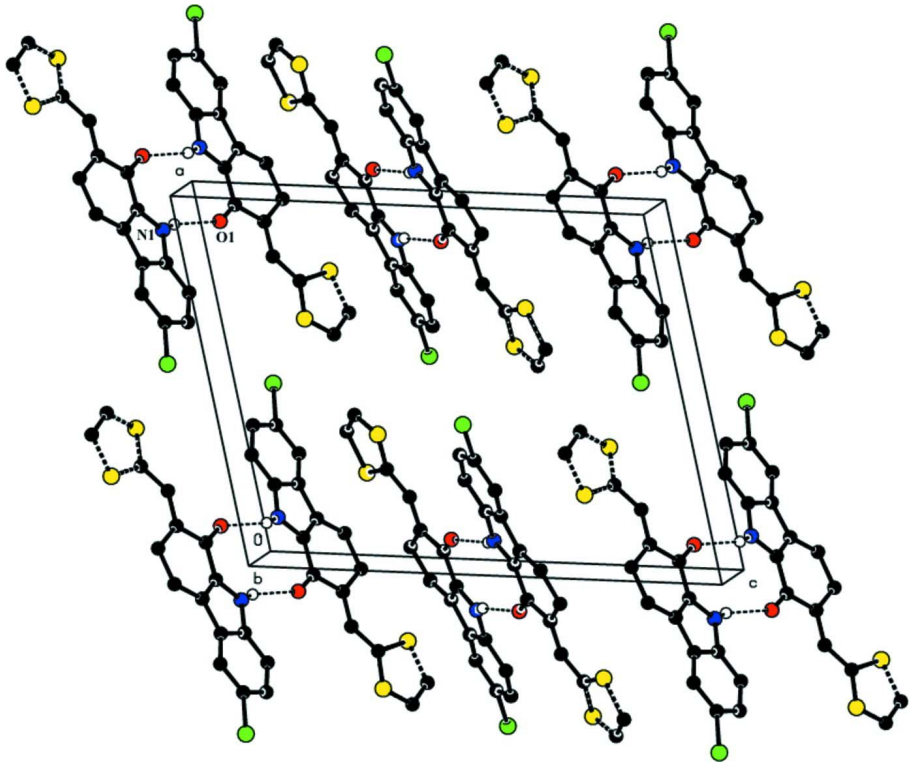

Figure 2

The crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

6-Bromo-2-[(*E*)-thiophen-2-ylmethylidene]-2,3,4,9-tetrahydro-1*H*- carbazol-1-one

Crystal data

$C_{17}H_{12}BrNOS$	a = 13.8655 (5) Å
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Monoclinic, $P2_1/c$	c = 17.4583 (7) Å
Hall symbol: -P 2ybc	β = 103.666 (2)°

V = 1483.76 (11) Å^3
Z = 4
F(000) = 720
D_x = 1.604 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1432 reflections
θ = 2.4–30.5°
μ = 2.91 mm^{-1}
T = 296 K
Block, yellow
0.21 × 0.17 × 0.16 mm

Data collection

Bruker SMART APEX CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.558, T_{max} = 0.628
12158 measured reflections
4487 independent reflections
1953 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 30.5°, θ_{min} = 2.4°
h = −19→19
k = −4→8
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
S = 0.85
4487 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
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.4371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Br1	1.44365 (3)	−0.32770 (7)	0.06412 (3)	0.0742 (2)	
S1	0.76193 (8)	−0.1866 (2)	0.24215 (7)	0.0665 (5)	0.843 (4)
C18′	0.76193 (8)	−0.1866 (2)	0.24215 (7)	0.0665 (5)	0.157 (4)
H18′	0.8144	−0.2822	0.2546	0.080*	0.157 (4)
O1	0.91041 (18)	0.3896 (4)	0.06209 (14)	0.0557 (6)	
N1	1.1050 (2)	0.2754 (5)	0.04571 (15)	0.0474 (7)	
H1	1.0940	0.4036	0.0258	0.057*	
C2	1.1893 (2)	0.1612 (5)	0.04737 (18)	0.0419 (8)	
C3	1.2698 (3)	0.2105 (6)	0.0147 (2)	0.0546 (10)	
H3	1.2722	0.3377	−0.0117	0.066*	
C4	1.3444 (3)	0.0657 (7)	0.0229 (2)	0.0569 (10)	

H4	1.3992	0.0949	0.0026	0.068*	
C5	1.3393 (2)	−0.1272 (6)	0.0619 (2)	0.0523 (9)	
C6	1.2619 (2)	−0.1797 (6)	0.09508 (19)	0.0458 (8)	
H6	1.2604	−0.3082	0.1209	0.055*	
C7	1.1855 (2)	−0.0306 (5)	0.08814 (16)	0.0401 (7)	
C8	1.0929 (2)	−0.0273 (5)	0.11198 (16)	0.0380 (7)	
C9	1.0491 (3)	−0.1861 (6)	0.1562 (2)	0.0556 (10)	
H9A	1.0982	−0.2242	0.2037	0.067*	
H9B	1.0334	−0.3129	0.1243	0.067*	
C10	0.9568 (3)	−0.1110 (6)	0.1789 (2)	0.0598 (10)	
H10A	0.9104	−0.2286	0.1706	0.072*	
H10B	0.9746	−0.0836	0.2352	0.072*	
C11	0.9014 (2)	0.0798 (5)	0.14016 (17)	0.0405 (7)	
C12	0.9501 (2)	0.2235 (6)	0.09254 (18)	0.0413 (8)	
C13	1.0475 (2)	0.1591 (5)	0.08458 (17)	0.0412 (8)	
C14	0.8096 (2)	0.1348 (6)	0.14535 (19)	0.0472 (8)	
H14	0.7854	0.2568	0.1174	0.057*	
C15	0.7412 (2)	0.0388 (6)	0.18652 (17)	0.0480 (9)	
C16	0.6513 (3)	−0.1697 (8)	0.2658 (2)	0.0711 (13)	
H16	0.6297	−0.2663	0.2984	0.085*	
C17	0.5980 (3)	−0.0032 (9)	0.2330 (3)	0.0820 (14)	
H17	0.5350	0.0233	0.2406	0.098*	
S1′	0.6432 (3)	0.1340 (6)	0.1851 (2)	0.0920 (14)	0.157 (4)
C18	0.6432 (3)	0.1340 (6)	0.1851 (2)	0.0920 (14)	0.843 (4)
H18	0.6164	0.2565	0.1589	0.110*	0.843 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0607 (3)	0.0682 (3)	0.1064 (4)	−0.0012 (2)	0.0451 (2)	−0.0058 (2)
S1	0.0530 (7)	0.0737 (10)	0.0782 (8)	−0.0023 (6)	0.0263 (6)	0.0248 (7)
C18′	0.0530 (7)	0.0737 (10)	0.0782 (8)	−0.0023 (6)	0.0263 (6)	0.0248 (7)
O1	0.0592 (14)	0.0422 (14)	0.0678 (15)	0.0038 (13)	0.0193 (12)	0.0176 (13)
N1	0.0558 (17)	0.0388 (16)	0.0505 (16)	−0.0049 (14)	0.0180 (13)	0.0134 (14)
C2	0.0544 (18)	0.0353 (18)	0.0381 (16)	−0.0101 (17)	0.0152 (14)	0.0008 (15)
C3	0.064 (2)	0.053 (2)	0.0515 (19)	−0.019 (2)	0.0240 (17)	0.0035 (18)
C4	0.058 (2)	0.064 (3)	0.057 (2)	−0.017 (2)	0.0289 (17)	−0.003 (2)
C5	0.0466 (18)	0.057 (2)	0.057 (2)	−0.0071 (18)	0.0210 (16)	−0.0063 (19)
C6	0.0471 (18)	0.044 (2)	0.0508 (18)	−0.0068 (17)	0.0199 (15)	0.0014 (17)
C7	0.0489 (17)	0.0386 (19)	0.0349 (15)	−0.0072 (16)	0.0141 (14)	−0.0016 (15)
C8	0.0455 (16)	0.0348 (18)	0.0352 (15)	−0.0046 (15)	0.0127 (13)	0.0018 (15)
C9	0.054 (2)	0.049 (2)	0.071 (2)	0.0043 (18)	0.0288 (18)	0.0206 (19)
C10	0.066 (2)	0.054 (2)	0.071 (2)	0.009 (2)	0.0374 (19)	0.023 (2)
C11	0.0510 (18)	0.0354 (18)	0.0364 (15)	−0.0037 (16)	0.0129 (14)	−0.0020 (15)
C12	0.0490 (18)	0.0353 (19)	0.0395 (16)	−0.0046 (16)	0.0099 (14)	−0.0004 (16)
C13	0.0471 (17)	0.0367 (19)	0.0408 (16)	−0.0073 (16)	0.0122 (14)	0.0006 (16)
C14	0.0522 (19)	0.044 (2)	0.0455 (18)	−0.0011 (17)	0.0112 (15)	0.0072 (16)
C15	0.0454 (17)	0.059 (2)	0.0402 (16)	−0.0049 (18)	0.0108 (14)	0.0017 (17)

C16	0.052 (2)	0.093 (4)	0.073 (3)	−0.014 (2)	0.022 (2)	0.016 (3)
C17	0.056 (2)	0.117 (4)	0.079 (3)	0.004 (3)	0.027 (2)	0.005 (3)
S1′	0.084 (2)	0.106 (3)	0.093 (2)	−0.006 (2)	0.0363 (18)	0.011 (2)
C18	0.084 (2)	0.106 (3)	0.093 (2)	−0.006 (2)	0.0363 (18)	0.011 (2)

Geometric parameters (Å, º)

Br1—C5	1.915 (4)	C8—C9	1.480 (4)
S1—C16	1.683 (4)	C9—C10	1.503 (4)
S1—C15	1.707 (4)	C9—H9A	0.9700
O1—C12	1.243 (4)	C9—H9B	0.9700
N1—C2	1.368 (4)	C10—C11	1.500 (5)
N1—C13	1.375 (4)	C10—H10A	0.9700
N1—H1	0.8789	C10—H10B	0.9700
C2—C3	1.403 (4)	C11—C14	1.343 (4)
C2—C7	1.411 (4)	C11—C12	1.495 (4)
C3—C4	1.361 (5)	C12—C13	1.448 (4)
C3—H3	0.9300	C14—C15	1.451 (4)
C4—C5	1.403 (5)	C14—H14	0.9300
C4—H4	0.9300	C15—S1′	1.480 (4)
C5—C6	1.376 (4)	C16—C17	1.333 (6)
C6—C7	1.400 (4)	C16—H16	0.9300
C6—H6	0.9300	C17—S1′	1.445 (6)
C7—C8	1.441 (4)	C17—H17	0.9300
C8—C13	1.366 (4)		

C16—S1—C15	92.6 (2)	H9A—C9—H9B	107.7
C2—N1—C13	107.5 (3)	C11—C10—C9	120.7 (3)
C2—N1—H1	124.1	C11—C10—H10A	107.1
C13—N1—H1	128.2	C9—C10—H10A	107.1
N1—C2—C3	129.2 (3)	C11—C10—H10B	107.1
N1—C2—C7	109.2 (3)	C9—C10—H10B	107.1
C3—C2—C7	121.5 (3)	H10A—C10—H10B	106.8
C4—C3—C2	117.7 (3)	C14—C11—C12	116.2 (3)
C4—C3—H3	121.1	C14—C11—C10	124.7 (3)
C2—C3—H3	121.1	C12—C11—C10	119.1 (3)
C3—C4—C5	120.6 (3)	O1—C12—C13	121.6 (3)
C3—C4—H4	119.7	O1—C12—C11	122.5 (3)
C5—C4—H4	119.7	C13—C12—C11	115.9 (3)
C6—C5—C4	123.1 (3)	C8—C13—N1	111.1 (3)
C6—C5—Br1	119.5 (3)	C8—C13—C12	124.8 (3)
C4—C5—Br1	117.3 (2)	N1—C13—C12	124.1 (3)
C5—C6—C7	116.8 (3)	C11—C14—C15	131.8 (3)
C5—C6—H6	121.6	C11—C14—H14	114.1
C7—C6—H6	121.6	C15—C14—H14	114.1
C6—C7—C2	120.1 (3)	C14—C15—S1′	121.8 (3)
C6—C7—C8	133.8 (3)	C14—C15—S1	126.0 (3)
C2—C7—C8	106.0 (3)	S1′—C15—S1	112.2 (2)

C13—C8—C7	106.3 (3)	C17—C16—S1	112.9 (3)
C13—C8—C9	123.6 (3)	C17—C16—H16	123.6
C7—C8—C9	130.1 (3)	S1—C16—H16	123.6
C8—C9—C10	113.8 (3)	C16—C17—S1′	116.6 (4)
C8—C9—H9A	108.8	C16—C17—H17	121.7
C10—C9—H9A	108.8	S1′—C17—H17	121.7
C8—C9—H9B	108.8	C17—S1′—C15	105.6 (3)
C10—C9—H9B	108.8		

C13—N1—C2—C3	178.8 (3)	C10—C11—C12—O1	−176.4 (3)
C13—N1—C2—C7	−0.2 (3)	C14—C11—C12—C13	−177.7 (3)
N1—C2—C3—C4	−178.3 (3)	C10—C11—C12—C13	2.9 (4)
C7—C2—C3—C4	0.6 (5)	C7—C8—C13—N1	−0.6 (3)
C2—C3—C4—C5	1.0 (5)	C9—C8—C13—N1	−180.0 (3)
C3—C4—C5—C6	−1.5 (6)	C7—C8—C13—C12	177.2 (3)
C3—C4—C5—Br1	175.9 (3)	C9—C8—C13—C12	−2.2 (5)
C4—C5—C6—C7	0.4 (5)	C2—N1—C13—C8	0.5 (4)
Br1—C5—C6—C7	−176.9 (2)	C2—N1—C13—C12	−177.4 (3)
C5—C6—C7—C2	1.1 (5)	O1—C12—C13—C8	−175.6 (3)
C5—C6—C7—C8	177.9 (3)	C11—C12—C13—C8	5.2 (4)
N1—C2—C7—C6	177.4 (3)	O1—C12—C13—N1	2.0 (5)
C3—C2—C7—C6	−1.6 (5)	C11—C12—C13—N1	−177.3 (3)
N1—C2—C7—C8	−0.2 (3)	C12—C11—C14—C15	−178.8 (3)
C3—C2—C7—C8	−179.3 (3)	C10—C11—C14—C15	0.6 (6)
C6—C7—C8—C13	−176.7 (3)	C11—C14—C15—S1′	178.2 (4)
C2—C7—C8—C13	0.5 (3)	C11—C14—C15—S1	−0.6 (6)
C6—C7—C8—C9	2.7 (6)	C16—S1—C15—C14	178.6 (3)
C2—C7—C8—C9	179.8 (3)	C16—S1—C15—S1′	−0.4 (3)
C13—C8—C9—C10	−8.5 (5)	C15—S1—C16—C17	0.8 (4)
C7—C8—C9—C10	172.2 (3)	S1—C16—C17—S1′	−1.1 (6)
C8—C9—C10—C11	16.1 (5)	C16—C17—S1′—C15	0.8 (5)
C9—C10—C11—C14	166.8 (4)	C14—C15—S1′—C17	−179.2 (3)
C9—C10—C11—C12	−13.8 (5)	S1—C15—S1′—C17	−0.2 (4)
C14—C11—C12—O1	3.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1	0.93	2.33	2.759 (4)	108
N1—H1···O1^{i}	0.88	2.00	2.804 (4)	151

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.