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4′-*tert*-Butyl-5-chloro-3*H*-spiro[1,3-benzothiazole-2,1′-cyclohexane]

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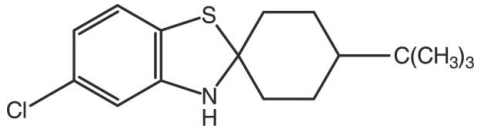
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.128; data-to-parameter ratio = 21.5.

In the title compound, $C_{16}H_{22}ClNS$, the nine-membered 2,3-dihydro-1,3-benzothiazole ring system is essentially planar, with a maximum deviation of 0.025 (2) Å for the N atom. Its plane is almost perpendicular to the main plane of the substituted cyclohexane ring, which adopts a chair conformation. In the crystal, the molecules are linked by C—H$\cdots\pi$ interactions.

Related literature

For the pharmacological activity of benzothiazole derivatives, see: Coudert *et al.* (1988); Karalı *et al.* (2010); Palmer *et al.* (1971). For the crystal structures of similar compounds, see, for example: Akkurt *et al.* (2010); Aryai *et al.* (1976); Karalı *et al.* (2010). For standard values of bond lengths, see: Allen *et al.* (1987). For details of ring-puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{16}H_{22}ClNS$
M_r = 295.87
Monoclinic, $P2_1/c$
a = 15.2810 (18) Å
b = 8.9830 (8) Å
c = 11.8750 (13) Å
β = 109.580 (3)°
V = 1535.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 K
0.27 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.915, T_{max} = 0.935
14074 measured reflections
3849 independent reflections
2330 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.128
S = 1.02
3849 reflections
179 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8*B*$\cdots$*Cg*1^{i}	0.97	2.84	3.796 (2)	169

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2411).

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Acta Cryst. (2012). E**68**, o1542 [doi:10.1107/S1600536812017539]

4′-*tert*-Butyl-5-chloro-3*H*-spiro[1,3-benzothiazole-2,1′-cyclohexane]

Mehmet Akkurt, Gökçe Cihan-Üstündağ, Gültaze Çapan, Yılmaz Dağdemir and Muhammad Nawaz Tahir

S1. Comment

The condensation of aldehydes and ketones with 2-aminothiophenoles lead to benzothiazolines and spirobenzothiazolines which are reported to exhibit antitubercular (Palmer *et al.*, 1971), analgesic (Coudert *et al.*, 1988) and antioxidant (Karalı *et al.*, 2010) properties. The reactivity of cyclic ketones towards 2-aminothiophenoles has also been examined and the structure of the end products has been discussed (Aryai *et al.*, 1976; Coudert *et al.*, 1988; Akkurt *et al.*, 2010; Karalı *et al.*, 2010). Prompted by the above observations, we report here the synthesis, spectroscopic and crystal structure of the title compound.

As shown in Fig. 1, the C7—C12 cyclohexane ring of the title compound adopts a chair conformation [puckering parameters (Cremer & Pople, 1975): Q_T = 0.564 (2) Å, θ = 176.5 (2) ° and φ = 4(4) °]. The mean plane of the 2,3-dihydro-1,3-benzothiazole ring system [max. deviation: -0.025 (2) Å for N1] is almost perpendicular with a dihedral angle of 89.39 (5) ° to the main plane formed by the C8,C9, C11 and C12 atoms of the cyclohexane ring. The bond lengths (Allen *et al.*, 1987) and bond angles are within the expected values.

The crystal packing is stabilized by C—H···π interactions (Table 1 and Fig. 2).

S2. Experimental

A mixture of 2-amino-4-chlorothiophenol (0.01 mol) and 4-*tert*-butylcyclohexanone (0.01 mol) in absolute ethanol (50 ml) was refluxed on a water bath for 8 h. The solvent was evaporated in a crystallizing dish at room temperature and the residue was recrystallized twice from ethanol, giving X-ray quality crystals [Yield: 24.3%, m.p.: 453–455 K]. Analysis calculated for $C_{16}H_{22}ClNS$: C 64.95, H 7.49, N 4.73%. Found: C 64.91, H 7.47, N 4.64%. Spectroscopic data for the title compound are given in the archive CIF.

S3. Refinement

The NH H atom was located in a difference Fourier map and freely refined. C-bound H atoms were placed in calculated positions and treated as riding atoms : C—H = 0.93, 0.96, 0.97 and 0.98 Å, for the aromatic, methyl, methylene and methine H atoms, respectively, with U_{iso}(H) = xU_{eq}(C), x = 1.5 for methyl H atoms and = 1.2 for other H atoms.

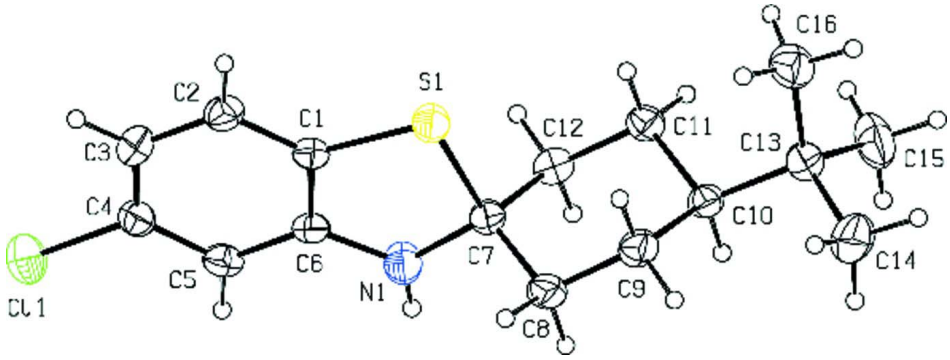

Figure 1

The molecular structure of the title molecule, with the atom numbering. Displacement ellipsoids are drawn at the 30% probability level.

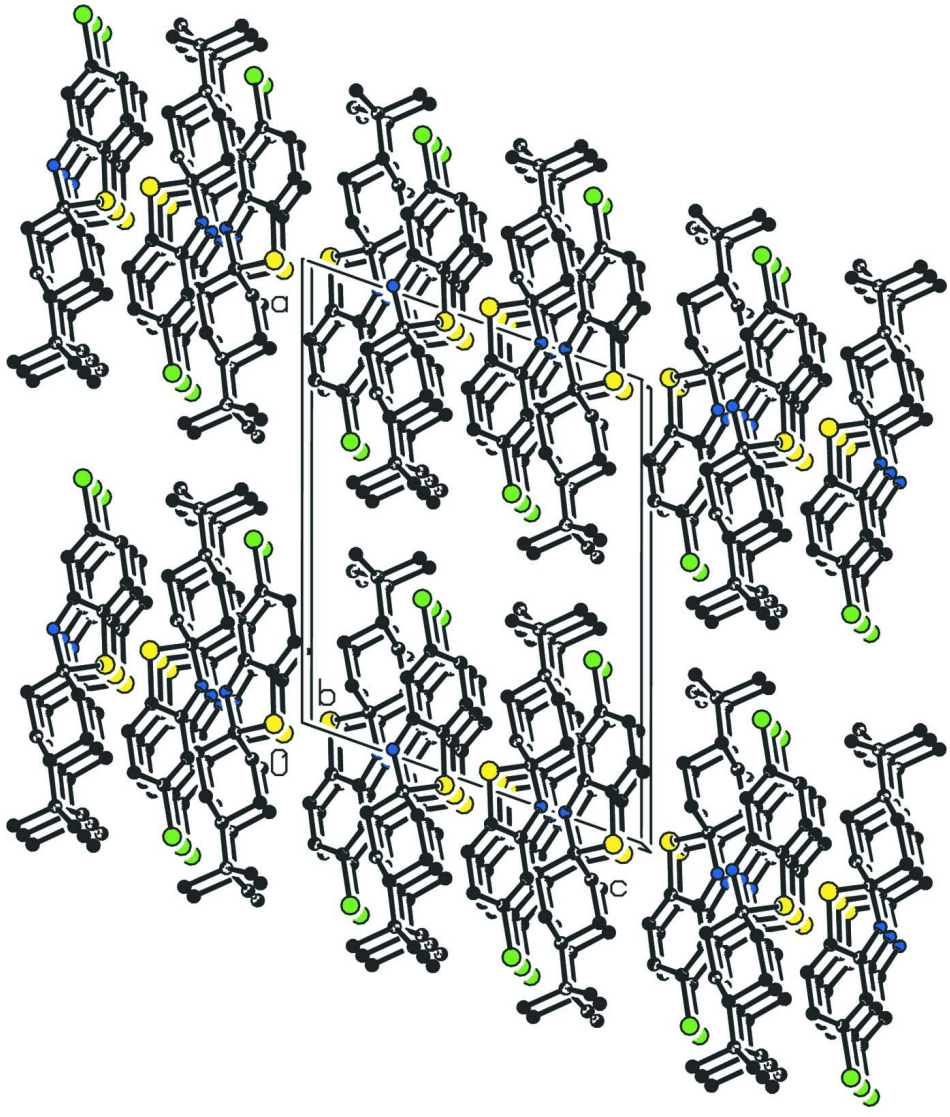

Figure 2

The crystal packing of the title compound viewing along *b* axis [H atoms have been omitted for clarity].

4′-*tert*-Butyl-5-chloro-3*H*-spiro[1,3-benzothiazole-2,1′- cyclohexane]

Crystal data

$C_{16}H_{22}ClNS$
$M_r = 295.87$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.2810\ (18)$ Å
$b = 8.9830\ (8)$ Å
$c = 11.8750\ (13)$ Å
$\beta = 109.580\ (3)°$
$V = 1535.8\ (3)$ Å^3
$Z = 4$
$F(000) = 632$
$D_x = 1.280$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 776 reflections
$\theta = 3.3–19.5°$
$\mu = 0.37$ mm^{-1}
$T = 296$ K
Prism, colourless
0.27 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.915$, $T_{max} = 0.935$
14074 measured reflections
3849 independent reflections
2330 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.7°$
$h = -20\rightarrow20$
$k = -11\rightarrow10$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.128$
$S = 1.02$
3849 reflections
179 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.2285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Experimental. Spectroscopic data for the title compound: IR (KBr) *v* = 3370 (N—H), 2962, 2912, 2862 (C—H), 1585, 1571, 1473, 1442 (C=C) cm^{-1}; 1*H*-NMR (DMSO-d6, 500 MHz) d= 0.83–0.86 (9*H*, m, 4′-C(CH3)3-cyc.), 0.95–1.02 (1*H*, m, CH/CH2-cyc.), 1.09–1.36 (2*H*, m, CH/CH2-cyc.), 1.58–1.72 (4*H*, m, CH/CH2-cyc.), 2.15–2.22 (2*H*, m, CH/CH2-cyc.), 6.40, 6.47 (1*H*, 2 d, J=2.0 Hz, H4-bt.), 6.50 (1*H*, dd, J=8.1, 2.0 Hz, H6-bt.), 6.90 (1*H*, d, J=7.8 Hz, H7-bt.), 6.73, 6.97 (1*H*, 2 s, NH) p.p.m. (cyc.=cyclohexane, bt.=benzothiazole).

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}
Cl1	−0.35486 (5)	0.80459 (8)	0.13722 (7)	0.0761 (3)
S1	0.02827 (4)	0.69814 (6)	0.07426 (5)	0.0503 (2)
N1	−0.00626 (14)	0.8895 (2)	0.2213 (2)	0.0628 (8)
C1	−0.08493 (14)	0.7159 (2)	0.07911 (17)	0.0369 (7)
C2	−0.16334 (16)	0.6409 (2)	0.0125 (2)	0.0474 (8)
C3	−0.24750 (16)	0.6684 (2)	0.0286 (2)	0.0515 (8)
C4	−0.25028 (16)	0.7710 (2)	0.1132 (2)	0.0469 (8)
C5	−0.17272 (16)	0.8482 (2)	0.1807 (2)	0.0447 (7)
C6	−0.08920 (15)	0.8210 (2)	0.16337 (18)	0.0390 (7)
C7	0.07535 (15)	0.8422 (2)	0.1936 (2)	0.0442 (7)
C8	0.11774 (16)	0.9705 (2)	0.1463 (2)	0.0519 (8)
C9	0.20566 (15)	0.9285 (2)	0.1218 (2)	0.0500 (8)
C10	0.27931 (14)	0.8647 (2)	0.23261 (18)	0.0408 (7)
C11	0.23620 (15)	0.7316 (2)	0.27578 (19)	0.0438 (7)
C12	0.14820 (15)	0.7730 (2)	0.30136 (19)	0.0467 (8)
C13	0.37389 (16)	0.8291 (2)	0.2176 (2)	0.0509 (8)
C14	0.4048 (2)	0.9596 (3)	0.1572 (3)	0.0845 (14)
C15	0.44715 (18)	0.8047 (3)	0.3408 (2)	0.0800 (11)
C16	0.36933 (18)	0.6896 (3)	0.1415 (2)	0.0651 (10)
H1N	−0.0005 (17)	0.955 (2)	0.2742 (16)	0.070 (8)*
H2	−0.16000	0.57120	−0.04380	0.0570*
H3	−0.30100	0.61850	−0.01690	0.0620*
H5	−0.17650	0.91750	0.23700	0.0540*
H8A	0.07240	1.00700	0.07300	0.0620*
H8B	0.13160	1.05100	0.20410	0.0620*
H9A	0.23040	1.01600	0.09520	0.0600*
H9B	0.19090	0.85550	0.05810	0.0600*
H10	0.29130	0.94100	0.29500	0.0490*
H11A	0.22180	0.65430	0.21530	0.0520*
H11B	0.28120	0.69160	0.34790	0.0520*
H12A	0.12260	0.68450	0.32520	0.0560*
H12B	0.16360	0.84290	0.36740	0.0560*
H14A	0.46750	0.94360	0.15950	0.1270*
H14B	0.40160	1.05020	0.19850	0.1270*
H14C	0.36470	0.96690	0.07550	0.1270*
H15A	0.50660	0.78790	0.33200	0.1200*
H15B	0.43040	0.71970	0.37820	0.1200*
H15C	0.45040	0.89120	0.38960	0.1200*
H16A	0.31930	0.69930	0.06700	0.0980*
H16B	0.35900	0.60370	0.18350	0.0980*
H16C	0.42680	0.67840	0.12620	0.0980*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0543 (4)	0.0816 (5)	0.1046 (6)	0.0027 (3)	0.0428 (4)	−0.0018 (4)
S1	0.0456 (3)	0.0510 (4)	0.0568 (4)	−0.0017 (3)	0.0203 (3)	−0.0182 (3)
N1	0.0467 (12)	0.0636 (14)	0.0770 (15)	−0.0030 (10)	0.0191 (11)	−0.0390 (12)
C1	0.0441 (12)	0.0319 (11)	0.0363 (11)	0.0025 (9)	0.0158 (9)	0.0017 (8)
C2	0.0533 (14)	0.0404 (12)	0.0483 (13)	−0.0035 (10)	0.0168 (11)	−0.0086 (10)
C3	0.0460 (14)	0.0488 (14)	0.0571 (15)	−0.0096 (11)	0.0139 (12)	−0.0054 (11)
C4	0.0438 (13)	0.0414 (12)	0.0586 (15)	0.0046 (10)	0.0214 (11)	0.0072 (10)
C5	0.0531 (14)	0.0361 (11)	0.0492 (13)	0.0061 (10)	0.0229 (11)	−0.0011 (9)
C6	0.0455 (13)	0.0295 (10)	0.0412 (12)	0.0022 (9)	0.0133 (10)	−0.0016 (9)
C7	0.0402 (13)	0.0395 (12)	0.0517 (13)	−0.0018 (9)	0.0139 (11)	−0.0117 (10)
C8	0.0483 (14)	0.0382 (12)	0.0580 (15)	0.0040 (10)	0.0030 (11)	0.0069 (10)
C9	0.0518 (14)	0.0434 (12)	0.0515 (14)	−0.0031 (10)	0.0131 (11)	0.0118 (10)
C10	0.0424 (12)	0.0352 (11)	0.0411 (12)	−0.0016 (9)	0.0091 (10)	−0.0016 (9)
C11	0.0465 (13)	0.0404 (12)	0.0400 (12)	0.0039 (10)	0.0087 (10)	0.0094 (9)
C12	0.0554 (15)	0.0414 (12)	0.0440 (13)	−0.0032 (10)	0.0176 (11)	−0.0010 (9)
C13	0.0451 (14)	0.0488 (13)	0.0572 (15)	0.0010 (10)	0.0151 (11)	−0.0043 (11)
C14	0.070 (2)	0.0732 (19)	0.126 (3)	−0.0153 (15)	0.0536 (19)	0.0001 (18)
C15	0.0468 (16)	0.105 (2)	0.077 (2)	0.0111 (15)	0.0061 (15)	−0.0186 (16)
C16	0.0638 (17)	0.0669 (16)	0.0687 (17)	0.0053 (13)	0.0278 (14)	−0.0127 (13)

Geometric parameters (Å, º)

Cl1—C4	1.741 (3)	C2—H2	0.9300
S1—C1	1.757 (2)	C3—H3	0.9300
S1—C7	1.875 (2)	C5—H5	0.9300
N1—C6	1.369 (3)	C8—H8A	0.9700
N1—C7	1.456 (3)	C8—H8B	0.9700
N1—H1N	0.844 (18)	C9—H9A	0.9700
C1—C2	1.371 (3)	C9—H9B	0.9700
C1—C6	1.393 (3)	C10—H10	0.9800
C2—C3	1.384 (4)	C11—H11A	0.9700
C3—C4	1.375 (3)	C11—H11B	0.9700
C4—C5	1.375 (3)	C12—H12A	0.9700
C5—C6	1.381 (3)	C12—H12B	0.9700
C7—C12	1.519 (3)	C14—H14A	0.9600
C7—C8	1.519 (3)	C14—H14B	0.9600
C8—C9	1.515 (3)	C14—H14C	0.9600
C9—C10	1.528 (3)	C15—H15A	0.9600
C10—C13	1.548 (3)	C15—H15B	0.9600
C10—C11	1.534 (3)	C15—H15C	0.9600
C11—C12	1.521 (3)	C16—H16A	0.9600
C13—C15	1.531 (3)	C16—H16B	0.9600
C13—C16	1.533 (3)	C16—H16C	0.9600
C13—C14	1.529 (4)		

C1—S1—C7	92.59 (10)	C7—C8—H8A	109.00
C6—N1—C7	118.31 (19)	C7—C8—H8B	109.00
C6—N1—H1N	122.4 (18)	C9—C8—H8A	109.00
C7—N1—H1N	119.2 (18)	C9—C8—H8B	109.00
C2—C1—C6	120.3 (2)	H8A—C8—H8B	108.00
S1—C1—C6	111.63 (16)	C8—C9—H9A	109.00
S1—C1—C2	128.03 (16)	C8—C9—H9B	109.00
C1—C2—C3	120.35 (19)	C10—C9—H9A	109.00
C2—C3—C4	118.6 (2)	C10—C9—H9B	109.00
Cl1—C4—C3	119.39 (19)	H9A—C9—H9B	108.00
Cl1—C4—C5	118.43 (17)	C9—C10—H10	107.00
C3—C4—C5	122.2 (2)	C11—C10—H10	107.00
C4—C5—C6	118.9 (2)	C13—C10—H10	107.00
C1—C6—C5	119.7 (2)	C10—C11—H11A	109.00
N1—C6—C1	114.0 (2)	C10—C11—H11B	109.00
N1—C6—C5	126.29 (19)	C12—C11—H11A	109.00
S1—C7—N1	103.38 (15)	C12—C11—H11B	109.00
N1—C7—C8	111.46 (17)	H11A—C11—H11B	108.00
S1—C7—C8	110.32 (15)	C7—C12—H12A	109.00
S1—C7—C12	109.96 (13)	C7—C12—H12B	109.00
C8—C7—C12	109.82 (19)	C11—C12—H12A	109.00
N1—C7—C12	111.75 (19)	C11—C12—H12B	109.00
C7—C8—C9	113.43 (16)	H12A—C12—H12B	108.00
C8—C9—C10	111.89 (18)	C13—C14—H14A	110.00
C9—C10—C11	107.78 (18)	C13—C14—H14B	109.00
C9—C10—C13	115.16 (18)	C13—C14—H14C	109.00
C11—C10—C13	113.56 (16)	H14A—C14—H14B	109.00
C10—C11—C12	112.56 (16)	H14A—C14—H14C	109.00
C7—C12—C11	112.28 (18)	H14B—C14—H14C	109.00
C10—C13—C15	109.36 (19)	C13—C15—H15A	110.00
C10—C13—C16	112.15 (19)	C13—C15—H15B	109.00
C14—C13—C16	108.1 (2)	C13—C15—H15C	110.00
C15—C13—C16	108.70 (18)	H15A—C15—H15B	110.00
C14—C13—C15	108.4 (2)	H15A—C15—H15C	109.00
C10—C13—C14	110.04 (18)	H15B—C15—H15C	109.00
C1—C2—H2	120.00	C13—C16—H16A	110.00
C3—C2—H2	120.00	C13—C16—H16B	109.00
C2—C3—H3	121.00	C13—C16—H16C	109.00
C4—C3—H3	121.00	H16A—C16—H16B	109.00
C4—C5—H5	121.00	H16A—C16—H16C	109.00
C6—C5—H5	121.00	H16B—C16—H16C	110.00

C7—S1—C1—C2	180.00 (19)	C4—C5—C6—N1	178.9 (2)
C7—S1—C1—C6	−0.14 (15)	C4—C5—C6—C1	−0.5 (3)
C1—S1—C7—N1	−1.11 (14)	S1—C7—C8—C9	−68.5 (2)
C1—S1—C7—C8	−120.40 (16)	N1—C7—C8—C9	177.21 (19)
C1—S1—C7—C12	118.33 (16)	C12—C7—C8—C9	52.8 (2)
C6—N1—C7—S1	2.3 (2)	S1—C7—C12—C11	69.25 (19)

C6—N1—C7—C8	120.8 (2)	N1—C7—C12—C11	−176.55 (16)
C6—N1—C7—C12	−115.9 (2)	C8—C7—C12—C11	−52.3 (2)
C7—N1—C6—C1	−2.6 (3)	C7—C8—C9—C10	−56.6 (2)
C7—N1—C6—C5	178.01 (19)	C8—C9—C10—C11	56.2 (2)
S1—C1—C2—C3	179.60 (16)	C8—C9—C10—C13	−175.93 (15)
C6—C1—C2—C3	−0.3 (3)	C9—C10—C11—C12	−56.7 (2)
S1—C1—C6—N1	1.5 (2)	C13—C10—C11—C12	174.45 (17)
S1—C1—C6—C5	−179.09 (15)	C9—C10—C13—C14	46.7 (2)
C2—C1—C6—N1	−178.61 (18)	C9—C10—C13—C15	165.71 (17)
C2—C1—C6—C5	0.8 (3)	C9—C10—C13—C16	−73.6 (2)
C1—C2—C3—C4	−0.6 (3)	C11—C10—C13—C14	171.7 (2)
C2—C3—C4—C5	0.9 (3)	C11—C10—C13—C15	−69.4 (2)
C2—C3—C4—Cl1	−178.66 (16)	C11—C10—C13—C16	51.3 (2)
Cl1—C4—C5—C6	179.20 (15)	C10—C11—C12—C7	56.6 (2)
C3—C4—C5—C6	−0.4 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···*Cg*1^{i}	0.97	2.84	3.796 (2)	169

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