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5-Chloro-4′-ethyl-3*H*-spiro[1,3-benzothiazole-2,1′-cyclohexane]

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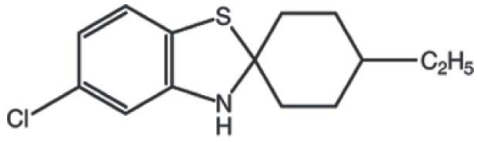
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.092; data-to-parameter ratio = 20.1.

In the title compound, $C_{14}H_{18}ClNS$, the 2,3-dihydro-1,3-thiazole ring adopts an envelope with the S,N-bound C atom at the flap and the cyclohexane ring adopts a chair conformation. In the crystal, N—H···S hydrogen bonds with $C(5)$ motifs connect the molecules into chains parallel to the c axis.

Related literature

For the pharmacological activity of benzothiazole derivatives, see: Coudert *et al.* (1988); Karalı *et al.* (2010); Palmer *et al.* (1971). For standard bond lengths, see: Allen *et al.* (1987). For the graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995). For ring-puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{14}H_{18}ClNS$
M_r = 267.81
Orthorhombic, $P2_12_12_1$
a = 8.989 (3) Å
b = 11.163 (4) Å
c = 13.722 (4) Å
V = 1376.9 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 296 K
0.35 × 0.28 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.872, T_{max} = 0.903
7077 measured reflections
3203 independent reflections
2724 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.092
S = 1.03
3203 reflections
159 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 1320 Freidel pairs
Flack parameter: 0.02 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···S1^{i}	0.84 (2)	2.84 (2)	3.669 (2)	168 (2)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5210).

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supplementary materials

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5-Chloro-4′-ethyl-3*H*-spiro[1,3-benzothiazole-2,1′-cyclohexane]

Mehmet Akkurt, Gökçe Cihan-Üstündağ, Gültaze Çapan, Sevim Türktekin-Çelikesir and Muhammad Nawaz Tahir

Comment

Efforts to design, synthesize and screen new molecules that mimic the actions of currently available chemotherapeutics have resulted in numerous promising candidates incorporating the benzothiazole moiety. Benzothiazolines and spiro-benzothiazolines, the cyclic products obtained by the condensation of aldehydes and ketones with 2-aminothiophenoles were previously reported to exhibit antitubercular (Palmer *et al.*, 1971), analgesic (Coudert *et al*., 1988) and antioxidant (Karalı *et al.*, 2010) properties. In this context, the title compound was prepared by the condensation of 4-ethylcyclo-hexanone with 2-amino-4-chlorothiophenol in an attempt to obtain a new molecule with antioxidant action and to establish its definite structure *via* analytical, spectroscopic and crystallographic data.

In the title compound (I), (Fig. 1), the S1/N1/C1/C6/C7 2,3-dihydro-1,3-thiazole ring adopts an envelope conformation with the C7 atom at the flap [puckering parameters (Cremer & Pople, 1975): Q(2) = 0.2817 (18) Å, φ(2) = 144.3 (4) °]. The C7—C12 cyclohexane ring adopts a chair conformation [puckering parameters: Q_T = 0.552 (2) Å, θ = 180.0 (2) ° and φ = 337 (7)°]. The bond lengths of (I) are within the expected values (Allen *et al.*, 1987).

In the crystal, molecules are linked by intermolecular N1—H1N···S1 hydrogen bonds (Table 1 and Figs. 2 & 3), forming C(5) motifs (Bernstein *et al.*, 1995) as chains parallel to the *c* axis.

Experimental

A mixture of 2-amino-4-chlorothiophenol (0.01 mol) and 4-ethylcyclohexanone (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 from ethanol. [Yield: 45.5%, m.p.: 381–383 K]. IR (KBr) ν = 3310 (N—H), 2960, 2916, 2893 (C—H), 1585, 1562, 1469, 1448 (C=C) cm^{-1}; ^{1}H-NMR (DMSO-d_6, 500 MHz) d = 0.85–0.87 (3*H*, m, 4′-CH_2—CH_3-cyc.), 1.00–1.16 (2*H*, m, CH/CH_2-cyc.), 1.17–1.34 (3*H*, m, 4′-CH_2—CH_3 and CH/CH_2-cyc.), 1.57–1.73 (4*H*, m, CH/CH_2-cyc.), 2.07–2.13 (2*H*, m, CH/CH_2-cyc.), 6.41, 6.47–6.50 (2*H*, d, J=2.0 Hz and m, H4 and H6-bt.), 6.90 (1*H*, d, J=8.3 Hz, H7-bt.), 6.74, 6.94 (1*H*, 2 s, NH) p.p.m. (Peaks at d 6.74 and 6.94 disappeared on D_2O exchange) (cyc.=cyclohexane, bt.=benzothiazole). Analysis calculated for $C_{14}H_{18}ClNS$: C 62.79, H 6.77, N 5.23%. Found: C 62.63, H 6.79, N 5.24%.

Refinement

C-bound H atoms were placed geometrically with the C—H distance of 0.93, 0.96, 0.97 and 0.98 Å, for the aromatic, methyl, methylene and methine H atoms, respectively and refined by using the riding model [U_{iso}(H) = xU_{eq}(C), x = 1.5 for methyl H and 1.2 for all other carbon-bound H atoms. The nitrogen-bound H atom were located in a difference Fourier map and refined freely with the constraint N—H = 0.86 (2) Å.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); 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* (Spek, 2009).

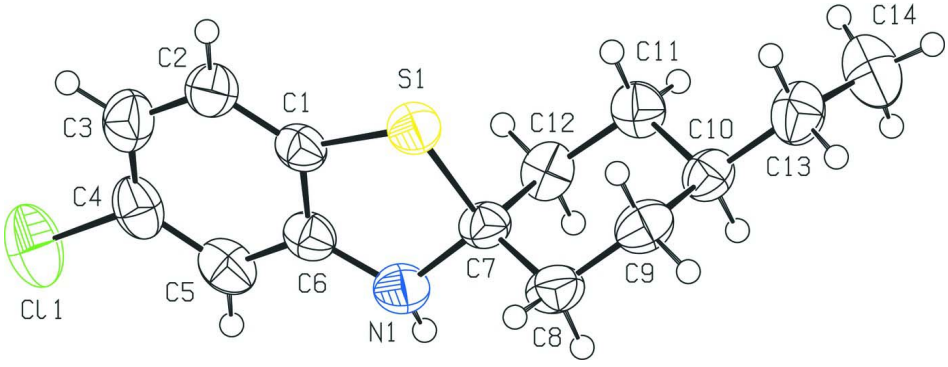

Figure 1

The title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

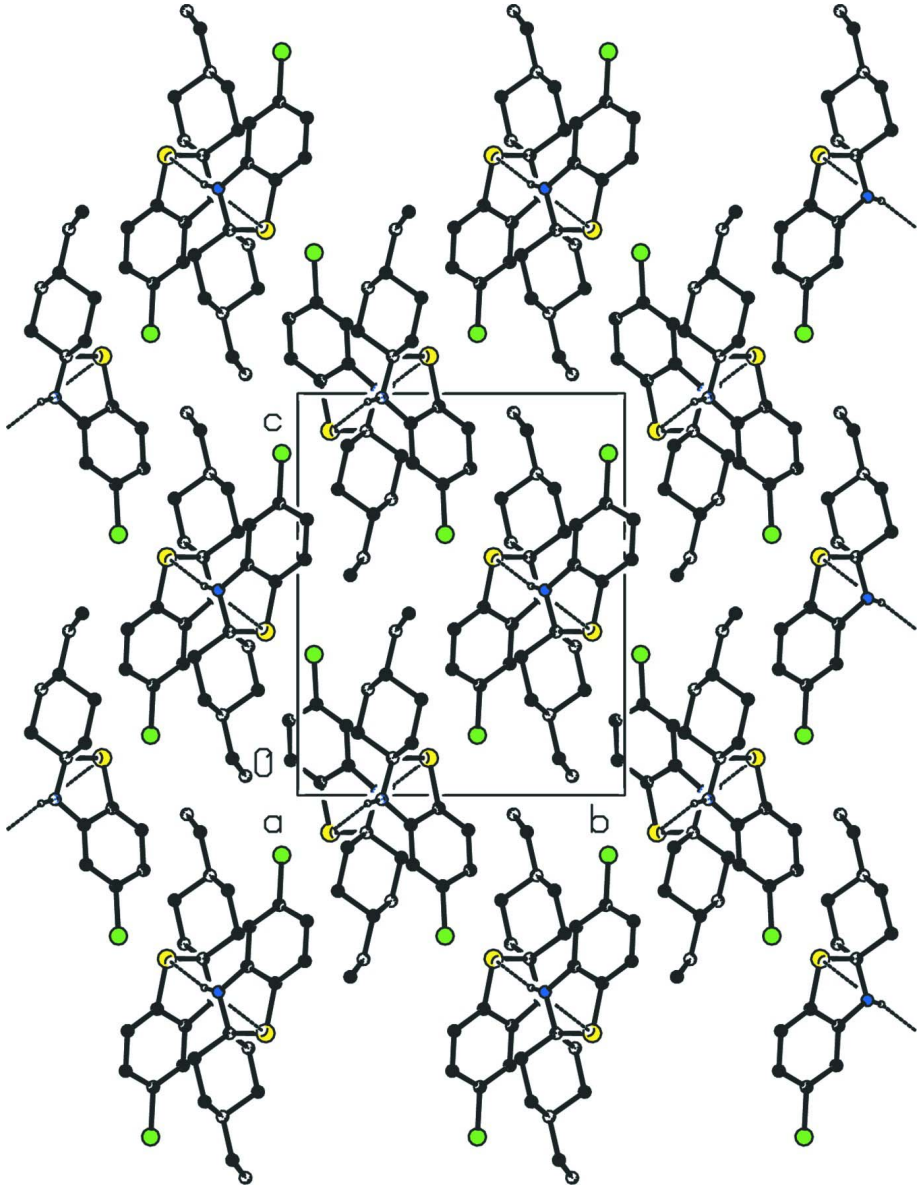

Figure 2

The packing and hydrogen bonding of the title molecule in the unit cell, viewing down *a* axis. H atoms not involved in hydrogen bonds have been omitted for clarity.

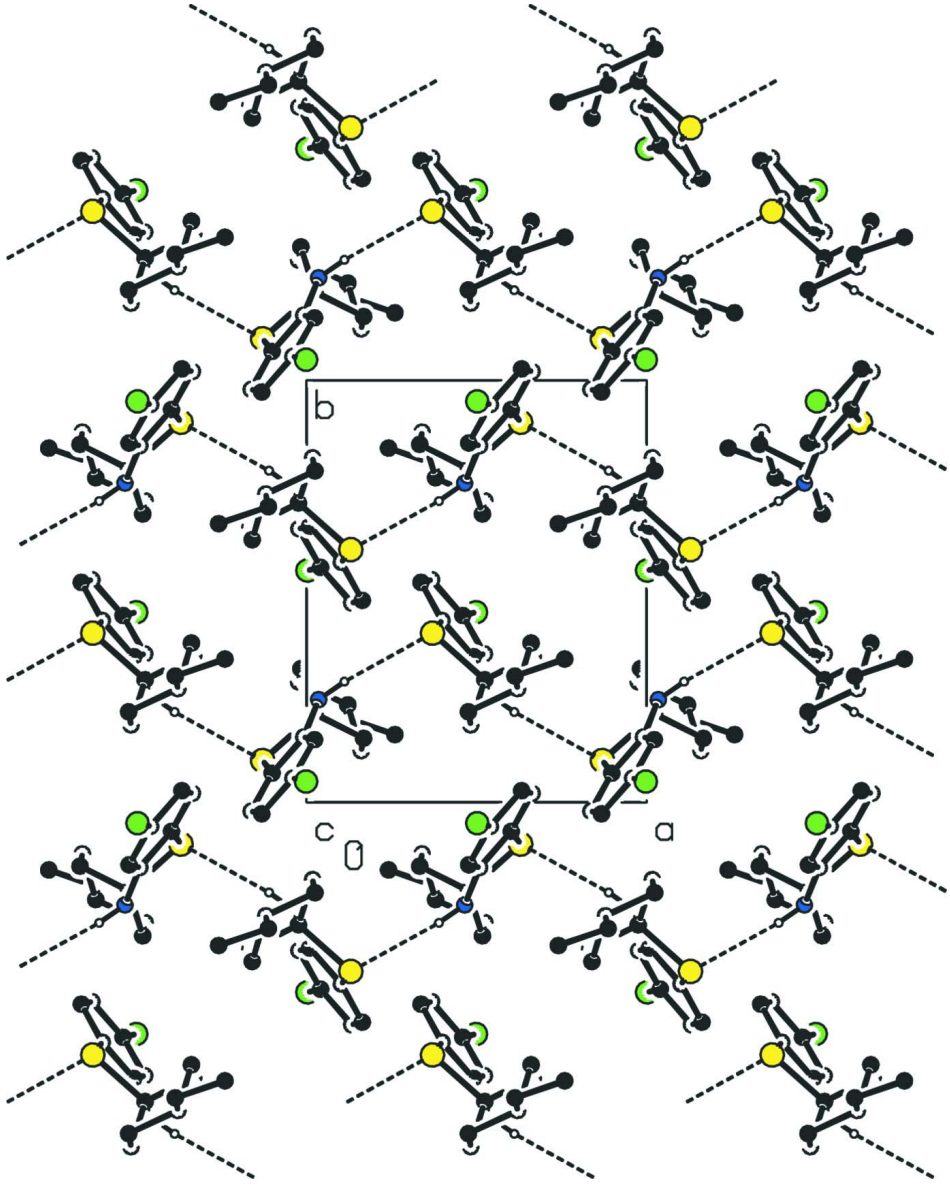

Figure 3

The packing and hydrogen bonding of the title molecule in the unit cell, viewing down *c* axis. H atoms not involved in hydrogen bonds have been omitted for clarity.

5-Chloro-4′-ethyl-3*H*-spiro[1,3-benzothiazole-2,1′-cyclohexane]

Crystal data

$C_{14}H_{18}ClNS$
$M_r = 267.81$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.989$ (3) Å
$b = 11.163$ (4) Å
$c = 13.722$ (4) Å
$V = 1376.9$ (8) Å^3
$Z = 4$

$F(000) = 568$
$D_x = 1.292$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 859 reflections
$\theta = 3.5$–20°
$\mu = 0.41$ mm^{-1}
$T = 296$ K
Prism, light yellow
0.35 × 0.28 × 0.25 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} = 0.872, T_{max} = 0.903
7077 measured reflections
3203 independent reflections
2724 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.9°, θ_{min} = 2.4°
h = −11→8
k = −14→10
l = −18→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.092
S = 1.03
3203 reflections
159 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
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 0.2606P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), 1320 Freidel pairs
Flack parameter: 0.02 (8)

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}
Cl1	0.49813 (9)	0.45066 (8)	−0.35059 (4)	0.0819 (3)
S1	0.37029 (6)	0.40096 (5)	0.09263 (4)	0.0481 (2)
N1	0.5350 (2)	0.25670 (18)	−0.01023 (14)	0.0529 (6)
C1	0.3980 (2)	0.43112 (18)	−0.03208 (14)	0.0430 (7)
C2	0.3365 (2)	0.5213 (2)	−0.08691 (16)	0.0540 (7)
C3	0.3676 (3)	0.5274 (2)	−0.18623 (17)	0.0597 (8)
C4	0.4593 (3)	0.4430 (2)	−0.22640 (16)	0.0547 (8)
C5	0.5230 (3)	0.3517 (2)	−0.17270 (16)	0.0527 (7)
C6	0.4912 (2)	0.34542 (18)	−0.07400 (14)	0.0437 (6)
C7	0.5242 (2)	0.29047 (17)	0.09277 (15)	0.0437 (6)
C8	0.4828 (3)	0.18328 (18)	0.15561 (16)	0.0534 (7)
C9	0.4758 (3)	0.21449 (19)	0.26303 (16)	0.0541 (7)
C10	0.6208 (3)	0.26917 (19)	0.30042 (15)	0.0470 (6)
C11	0.6605 (2)	0.3776 (2)	0.23844 (15)	0.0506 (7)
C12	0.6673 (2)	0.3484 (2)	0.12979 (15)	0.0495 (7)

C13	0.6130 (3)	0.2992 (2)	0.40837 (16)	0.0602 (8)
C14	0.7593 (3)	0.3396 (3)	0.4523 (2)	0.0791 (10)
H1N	0.611 (2)	0.214 (2)	−0.0203 (19)	0.078 (9)*
H2	0.27450	0.57770	−0.05800	0.0650*
H3	0.32680	0.58780	−0.22450	0.0720*
H5	0.58560	0.29600	−0.20200	0.0630*
H8A	0.38670	0.15290	0.13500	0.0640*
H8B	0.55560	0.12030	0.14590	0.0640*
H9A	0.45400	0.14260	0.30000	0.0650*
H9B	0.39520	0.27080	0.27370	0.0650*
H10	0.69960	0.20940	0.29160	0.0560*
H11A	0.75630	0.40850	0.25920	0.0610*
H11B	0.58700	0.43990	0.24900	0.0610*
H12A	0.68540	0.42150	0.09350	0.0590*
H12B	0.75000	0.29450	0.11790	0.0590*
H13A	0.53990	0.36200	0.41780	0.0720*
H13B	0.57860	0.22900	0.44340	0.0720*
H14A	0.83630	0.28400	0.43480	0.1190*
H14B	0.75030	0.34280	0.52190	0.1190*
H14C	0.78410	0.41770	0.42790	0.1190*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0729 (4)	0.1232 (6)	0.0495 (3)	−0.0171 (5)	0.0012 (3)	0.0056 (3)
S1	0.0423 (3)	0.0527 (3)	0.0492 (3)	0.0097 (3)	0.0031 (2)	−0.0056 (2)
N1	0.0541 (12)	0.0517 (11)	0.0528 (10)	0.0153 (10)	0.0027 (9)	−0.0101 (8)
C1	0.0378 (11)	0.0448 (12)	0.0464 (11)	−0.0016 (9)	−0.0028 (8)	−0.0087 (8)
C2	0.0495 (12)	0.0538 (13)	0.0586 (13)	0.0064 (10)	−0.0104 (11)	−0.0055 (11)
C3	0.0562 (13)	0.0646 (15)	0.0582 (13)	−0.0029 (13)	−0.0128 (12)	0.0067 (11)
C4	0.0476 (13)	0.0704 (15)	0.0462 (11)	−0.0142 (12)	−0.0063 (9)	−0.0003 (11)
C5	0.0423 (11)	0.0642 (14)	0.0517 (12)	−0.0016 (11)	0.0036 (10)	−0.0130 (11)
C6	0.0356 (10)	0.0465 (11)	0.0489 (11)	−0.0031 (9)	−0.0018 (9)	−0.0076 (9)
C7	0.0421 (11)	0.0398 (10)	0.0492 (11)	0.0056 (9)	0.0007 (10)	−0.0034 (9)
C8	0.0575 (13)	0.0375 (11)	0.0653 (14)	−0.0031 (10)	−0.0026 (12)	−0.0005 (9)
C9	0.0580 (14)	0.0426 (11)	0.0618 (13)	−0.0060 (11)	0.0061 (11)	0.0093 (10)
C10	0.0444 (11)	0.0463 (11)	0.0502 (11)	0.0066 (10)	0.0034 (10)	0.0035 (9)
C11	0.0450 (12)	0.0530 (13)	0.0537 (12)	−0.0103 (10)	−0.0018 (9)	0.0023 (10)
C12	0.0386 (11)	0.0559 (13)	0.0540 (12)	−0.0016 (10)	0.0030 (9)	0.0083 (10)
C13	0.0590 (14)	0.0690 (15)	0.0525 (13)	0.0078 (13)	0.0031 (12)	0.0082 (12)
C14	0.0742 (18)	0.104 (2)	0.0591 (15)	0.0009 (18)	−0.0082 (14)	−0.0086 (16)

Geometric parameters (Å, º)

Cl1—C4	1.742 (2)	C13—C14	1.515 (4)
S1—C1	1.762 (2)	C2—H2	0.9300
S1—C7	1.854 (2)	C3—H3	0.9300
N1—C6	1.379 (3)	C5—H5	0.9300
N1—C7	1.466 (3)	C8—H8A	0.9700
N1—H1N	0.84 (2)	C8—H8B	0.9700

C1—C6	1.396 (3)	C9—H9A	0.9700
C1—C2	1.373 (3)	C9—H9B	0.9700
C2—C3	1.393 (3)	C10—H10	0.9800
C3—C4	1.368 (3)	C11—H11A	0.9700
C4—C5	1.382 (3)	C11—H11B	0.9700
C5—C6	1.386 (3)	C12—H12A	0.9700
C7—C8	1.521 (3)	C12—H12B	0.9700
C7—C12	1.527 (3)	C13—H13A	0.9700
C8—C9	1.516 (3)	C13—H13B	0.9700
C9—C10	1.528 (4)	C14—H14A	0.9600
C10—C11	1.522 (3)	C14—H14B	0.9600
C10—C13	1.520 (3)	C14—H14C	0.9600
C11—C12	1.527 (3)		

C1—S1—C7	91.30 (9)	C6—C5—H5	121.00
C6—N1—C7	114.09 (17)	C7—C8—H8A	109.00
C6—N1—H1N	122.2 (17)	C7—C8—H8B	109.00
C7—N1—H1N	110.9 (18)	C9—C8—H8A	109.00
S1—C1—C2	127.99 (16)	C9—C8—H8B	109.00
S1—C1—C6	110.75 (14)	H8A—C8—H8B	108.00
C2—C1—C6	121.23 (18)	C8—C9—H9A	109.00
C1—C2—C3	119.4 (2)	C8—C9—H9B	109.00
C2—C3—C4	118.8 (2)	C10—C9—H9A	109.00
Cl1—C4—C5	118.36 (18)	C10—C9—H9B	109.00
C3—C4—C5	122.9 (2)	H9A—C9—H9B	108.00
Cl1—C4—C3	118.77 (18)	C9—C10—H10	108.00
C4—C5—C6	118.2 (2)	C11—C10—H10	108.00
N1—C6—C5	126.69 (19)	C13—C10—H10	108.00
N1—C6—C1	113.71 (17)	C10—C11—H11A	109.00
C1—C6—C5	119.46 (19)	C10—C11—H11B	109.00
S1—C7—C12	110.33 (14)	C12—C11—H11A	109.00
N1—C7—C8	111.13 (16)	C12—C11—H11B	109.00
S1—C7—C8	109.97 (14)	H11A—C11—H11B	108.00
C8—C7—C12	110.53 (17)	C7—C12—H12A	109.00
N1—C7—C12	111.96 (16)	C7—C12—H12B	109.00
S1—C7—N1	102.68 (13)	C11—C12—H12A	109.00
C7—C8—C9	112.37 (17)	C11—C12—H12B	109.00
C8—C9—C10	112.5 (2)	H12A—C12—H12B	108.00
C9—C10—C13	112.1 (2)	C10—C13—H13A	109.00
C11—C10—C13	112.33 (18)	C10—C13—H13B	109.00
C9—C10—C11	109.28 (18)	C14—C13—H13A	109.00
C10—C11—C12	112.66 (18)	C14—C13—H13B	109.00
C7—C12—C11	112.43 (16)	H13A—C13—H13B	108.00
C10—C13—C14	114.4 (2)	C13—C14—H14A	109.00
C1—C2—H2	120.00	C13—C14—H14B	110.00
C3—C2—H2	120.00	C13—C14—H14C	109.00
C2—C3—H3	121.00	H14A—C14—H14B	110.00
C4—C3—H3	121.00	H14A—C14—H14C	109.00
C4—C5—H5	121.00	H14B—C14—H14C	109.00

C7—S1—C1—C2	−169.63 (19)	Cl1—C4—C5—C6	−179.63 (18)
C7—S1—C1—C6	12.78 (15)	C3—C4—C5—C6	0.5 (4)
C1—S1—C7—N1	−22.42 (13)	C4—C5—C6—N1	175.0 (2)
C1—S1—C7—C8	−140.76 (15)	C4—C5—C6—C1	−0.6 (3)
C1—S1—C7—C12	97.06 (15)	S1—C7—C8—C9	−68.9 (2)
C6—N1—C7—S1	28.68 (19)	N1—C7—C8—C9	178.09 (19)
C6—N1—C7—C8	146.21 (18)	C12—C7—C8—C9	53.2 (3)
C6—N1—C7—C12	−89.7 (2)	S1—C7—C12—C11	69.5 (2)
C7—N1—C6—C1	−21.5 (2)	N1—C7—C12—C11	−176.80 (17)
C7—N1—C6—C5	162.7 (2)	C8—C7—C12—C11	−52.3 (2)
S1—C1—C2—C3	−177.34 (17)	C7—C8—C9—C10	−56.0 (3)
C6—C1—C2—C3	0.0 (3)	C8—C9—C10—C11	55.3 (2)
S1—C1—C6—N1	2.0 (2)	C8—C9—C10—C13	−179.54 (18)
S1—C1—C6—C5	178.12 (17)	C9—C10—C11—C12	−54.5 (2)
C2—C1—C6—N1	−175.77 (18)	C13—C10—C11—C12	−179.53 (19)
C2—C1—C6—C5	0.3 (3)	C9—C10—C13—C14	172.9 (2)
C1—C2—C3—C4	−0.1 (3)	C11—C10—C13—C14	−63.6 (3)
C2—C3—C4—C5	−0.1 (4)	C10—C11—C12—C7	54.5 (2)
C2—C3—C4—Cl1	179.98 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···S1^{i}	0.84 (2)	2.84 (2)	3.669 (2)	168 (2)

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