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# 2-Anilino-3-(2-hydroxypropyl)-4-methyl-1,3-thiazol-3-ium chloride

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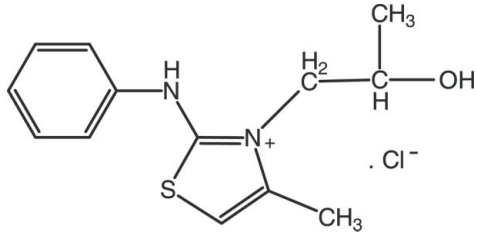
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.032; $wR$ factor = 0.084; data-to-parameter ratio = 15.9.

In the title compound, $C_{13}H_{17}N_2OS^+\cdot Cl^-$, the thiazolium ring mean plane makes a dihedral angle of 55.46 (9)° with the benzene ring. In the propanol group, the N—C—C—C and N—C—C—O torsion angles are 172.58 (15) and 52.9 (2)°, respectively, and the S—C—C—C torsion angle is 178.99 (18)°. In the crystal, molecules are linked by O—H···Cl and N—H···Cl hydrogen bonds, forming zigzag chains along [001]. There is also a C—H···Cl interaction present.

## Related literature

The title compound was prepared as part of an ongoing investigation into the synthesis and biological properties of thiazole compounds: see; Abdel-Wahab *et al.* (2009); Baia *et al.* (2008); Lesyk *et al.* (2007); Mohamed *et al.* (2012*a*,*b*); Potikha *et al.* (2008); Shiradkar *et al.* (2007); Soliman *et al.* (2012); Wu & Yang (2007). For related structures, see: Lynch & McClenaghan (2004); Liu *et al.* (2011); Wang (2011).




## Experimental

### Crystal data

$C_{13}H_{17}N_2OS^+\cdot Cl^-$
$M_r$ = 284.81
Monoclinic, $P2_1/c$
$a$ = 11.7570 (4) Å
$b$ = 12.2477 (4) Å
$c$ = 10.2954 (3) Å
$\beta$ = 106.532 (1)°
$V$ = 1421.21 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.41 mm$^{-1}$
$T$ = 296 K
0.35 × 0.22 × 0.20 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.898, $T_{max}$ = 0.922
10535 measured reflections
2641 independent reflections
2172 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
$S$ = 1.03
2641 reflections
166 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···Cl1 | 0.82 | 2.36 | 3.1681 (16) | 169 |
| N1—H1···Cl1$^{i}$ | 0.86 | 2.34 | 3.1675 (14) | 163 |
| C11—H11$A$···Cl1$^{i}$ | 0.97 | 2.81 | 3.6440 (19) | 144 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2431).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1881–o1882 [doi:10.1107/S1600536812023197]

## 2-Anilino-3-(2-hydroxypropyl)-4-methyl-1,3-thiazol-3-ium chloride

**Shaaban K. Mohamed, Mehmet Akkurt, Muhammad N. Tahir, Antar A. Abdelhamid and Ali N. Khalilov**

### Comment

Natural compounds such as, bistratamide H, archazolid A & B, siomycin A, didmolamide A, scleritodermin A, *etc*. (Wu & Yang, 2007) and thiamine (vitamin B1) (Baia *et al.*, 2008), were found to have a thiazol ring system. In addition, thiazole compounds have been reported to exhibit different pharmaceutical properties, for example antibacterial, antifungal (Abdel-Wahab *et al.*, 2009), antitubercular (Shiradkar *et al.*, 2007), anticancer (Lesyk *et al.*, 2007). These compounds have been synthesized using different methods (Potikha *et al.*, 2008). Further to our interest of bioactive compounds (Mohamed *et al.*, 2012*a,b*; Soliman *et al.*, 2012) we were interested in synthesizing new amino-thiazole derivatives *via* a one pot reaction protocol. We report herein on the synthesis and crystal structure of the title compound.

In the title compound, (Fig. 1), the dihedral angle between the thiazole ring (S1/N2/C7–C9) and the benzene ring (C1–C6) is 55.46 (9)°. The thiazolium ring is essentialy co-planar with the methyl group which is attached to it, with torsion angle S1—C9—C8—C10 being 178.99 (18)°. In the propanol group, torsion angles N2–C11–C12–C13 and N2–C11–C12–O1 are 172.58 (15) and 52.9 (2)°, respectively. Bond lengths and angles have normal values and are comparable to those reported for similar structures (Lynch & McClenaghan, 2004; Liu *et al.*, 2011; Wang, 2011).

In the crystal, molecules are linked by O-H···Cl, N—H···Cl and C—H···Cl hydrogen bonds, into infinite zigzag chains propagating along the [001] direction (Table 1, Fig. 2).

### Experimental

A mixture of 75 mg (1 mmol) 1-aminopropan-2-ol, 135 mg (1 mmol) phenyl isothiocyanate and 93 mg (1 mmol) 1-chloropropan-2-one in 50 ml ethanol was refluxed at 351 K. The reaction was monitored by TLC until completion after four hours then cooled to room temperature. The resulting solid was filtered off, dried under vacuum and recrystallized from ethanol to afford colourless crystals suitable for X-ray analysis [Yield 79%; M.p. 419 K].

### Refinement

The H atoms were located in a difference Fourier map. In the final cycles of refinement they were included in calculated poitions and refined using a riding model: N—H = 0.86 Å and C—H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.97 Å (methylene) and 0.98 Å (methine), with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl groups and = 1.2$U_{eq}$(C,*N*) for other H atoms.

### Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Spek, 2009).

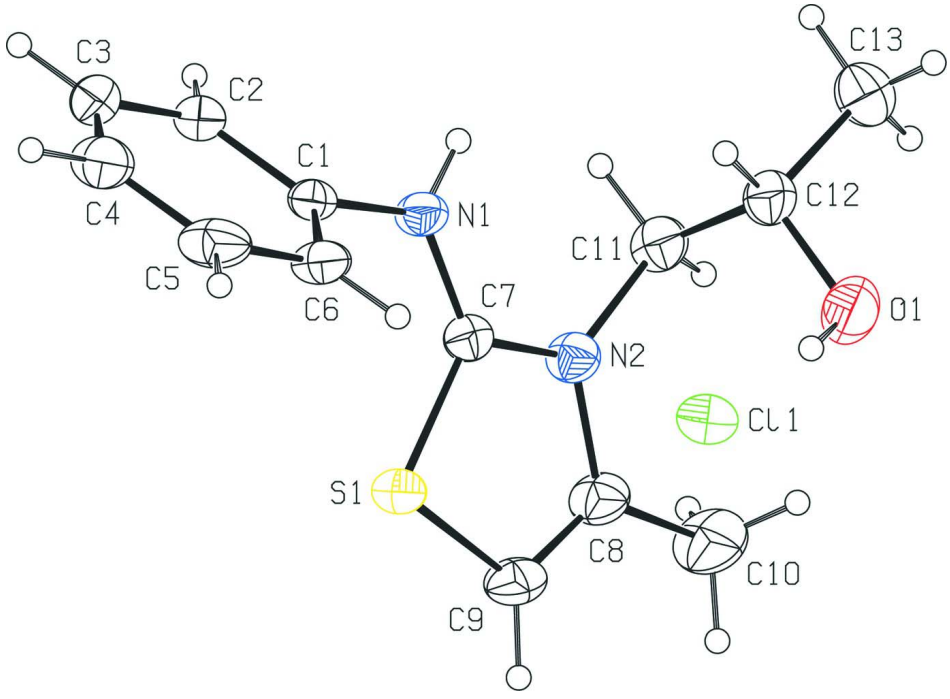


**Figure 1**

The molecular structure and atom-numbering scheme for the title compound. Displacement ellipsoids are drawn at the 30% probability level.

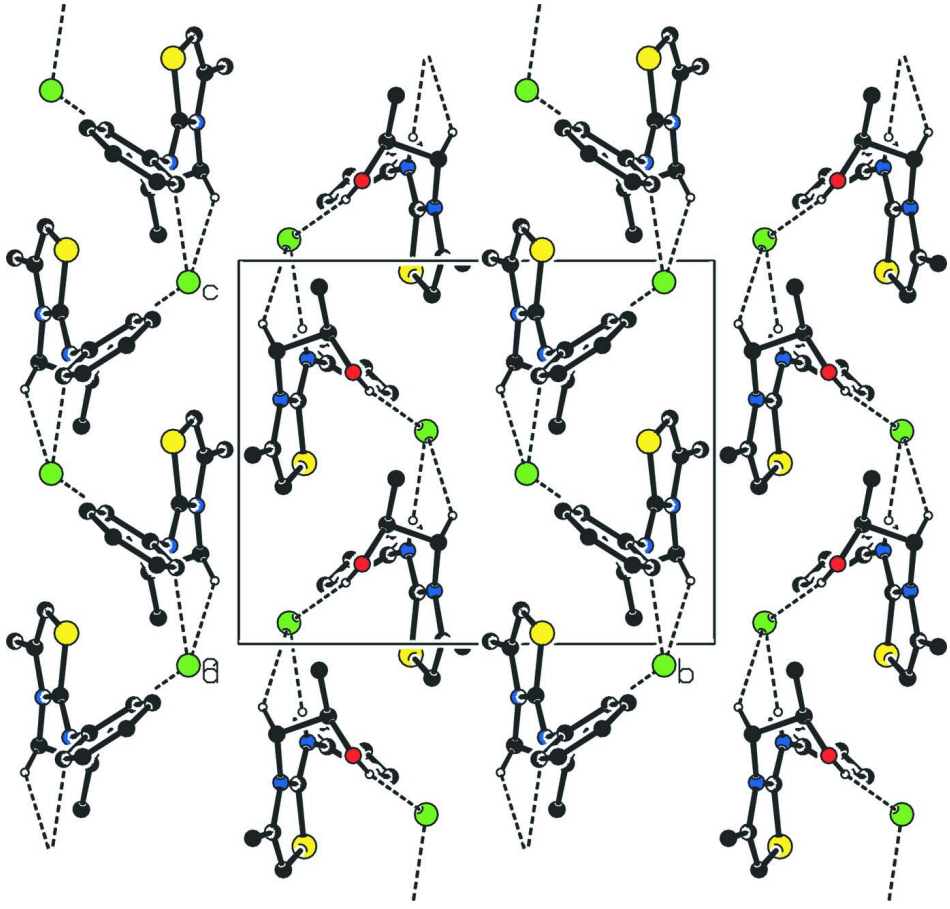


**Figure 2**

The crystal packing of the title compound, viewing along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

### 2-Anilino-3-(2-hydroxypropyl)-4-methyl-1,3-thiazol-3-ium chloride

*Crystal data*

$C_{13}H_{17}N_2OS^+\cdot Cl^-$
$M_r = 284.81$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.7570\ (4)$ Å
$b = 12.2477\ (4)$ Å
$c = 10.2954\ (3)$ Å
$\beta = 106.532\ (1)°$
$V = 1421.21\ (8)$ Å$^3$
$Z = 4$
$F(000) = 600$
$D_x = 1.331$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 447 reflections
$\theta = 3.5–21.2°$
$\mu = 0.41$ mm$^{-1}$
$T = 296$ K
Rod, colourless
0.35 × 0.22 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.81 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.898$, $T_{max} = 0.922$
10535 measured reflections
2641 independent reflections
2172 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.024
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.5°
$h$ = −14→11
$k$ = −14→14
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
$S$ = 1.03
2641 reflections
166 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
$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.3249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 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 | 0.53335 (4) | 0.36209 (4) | −0.02819 (4) | 0.0436 (2) |
| O1 | 0.92376 (12) | 0.25939 (14) | 0.20894 (15) | 0.0722 (6) |
| N1 | 0.58597 (12) | 0.35477 (12) | 0.24335 (13) | 0.0424 (4) |
| N2 | 0.73113 (12) | 0.41117 (12) | 0.13880 (14) | 0.0447 (5) |
| C1 | 0.47013 (14) | 0.31414 (14) | 0.23234 (15) | 0.0382 (5) |
| C2 | 0.40120 (15) | 0.36823 (15) | 0.30052 (17) | 0.0455 (6) |
| C3 | 0.29021 (17) | 0.3281 (2) | 0.29410 (19) | 0.0586 (7) |
| C4 | 0.24821 (17) | 0.2359 (2) | 0.22085 (19) | 0.0673 (8) |
| C5 | 0.31707 (18) | 0.18174 (19) | 0.15336 (18) | 0.0612 (7) |
| C6 | 0.42873 (16) | 0.22021 (15) | 0.15893 (16) | 0.0471 (6) |
| C7 | 0.62227 (15) | 0.37561 (13) | 0.13445 (16) | 0.0384 (5) |
| C8 | 0.74511 (17) | 0.42898 (16) | 0.00903 (19) | 0.0522 (7) |
| C9 | 0.64774 (18) | 0.40625 (15) | −0.08878 (19) | 0.0527 (7) |
| C10 | 0.8594 (2) | 0.4705 (2) | −0.0071 (2) | 0.0812 (9) |
| C11 | 0.82819 (15) | 0.41979 (16) | 0.26481 (18) | 0.0509 (6) |
| C12 | 0.88729 (16) | 0.31168 (18) | 0.31206 (19) | 0.0544 (7) |
| C13 | 0.99588 (18) | 0.3309 (2) | 0.4314 (2) | 0.0775 (9) |
| Cl1 | 0.71127 (4) | 0.10568 (4) | 0.05541 (4) | 0.0553 (2) |
| H1 | 0.63390 | 0.36620 | 0.32250 | 0.0510* |
| H1A | 0.86790 | 0.22510 | 0.16010 | 0.1080* |
| H2 | 0.42940 | 0.43100 | 0.35010 | 0.0550* |
| H3 | 0.24340 | 0.36390 | 0.33990 | 0.0700* |
| H4 | 0.17300 | 0.20970 | 0.21670 | 0.0810* |

| | | | | |
|---|---|---|---|---|
| H5 | 0.28820 | 0.11910 | 0.10390 | 0.0730* |
| H6 | 0.47560 | 0.18360 | 0.11400 | 0.0560* |
| H9 | 0.64160 | 0.41330 | −0.18050 | 0.0630* |
| H10A | 0.85460 | 0.47390 | −0.10170 | 0.1220* |
| H10B | 0.92260 | 0.42230 | 0.03820 | 0.1220* |
| H10C | 0.87460 | 0.54220 | 0.03170 | 0.1220* |
| H11A | 0.79720 | 0.44960 | 0.33520 | 0.0610* |
| H11B | 0.88720 | 0.47040 | 0.25100 | 0.0610* |
| H12 | 0.83160 | 0.26440 | 0.34050 | 0.0650* |
| H13A | 1.05130 | 0.37610 | 0.40350 | 0.1160* |
| H13B | 1.03240 | 0.26220 | 0.46350 | 0.1160* |
| H13C | 0.97260 | 0.36660 | 0.50290 | 0.1160* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0486 (3) | 0.0486 (3) | 0.0332 (2) | −0.0003 (2) | 0.0112 (2) | 0.0015 (2) |
| O1 | 0.0544 (8) | 0.0909 (12) | 0.0737 (10) | 0.0018 (8) | 0.0221 (8) | −0.0187 (8) |
| N1 | 0.0389 (7) | 0.0577 (9) | 0.0305 (7) | −0.0068 (7) | 0.0095 (6) | −0.0046 (6) |
| N2 | 0.0429 (8) | 0.0501 (9) | 0.0424 (8) | −0.0073 (7) | 0.0145 (6) | 0.0013 (6) |
| C1 | 0.0368 (9) | 0.0496 (10) | 0.0277 (8) | −0.0008 (8) | 0.0083 (7) | 0.0037 (7) |
| C2 | 0.0466 (10) | 0.0562 (11) | 0.0339 (9) | 0.0062 (8) | 0.0120 (8) | 0.0041 (8) |
| C3 | 0.0417 (10) | 0.0936 (16) | 0.0433 (11) | 0.0091 (11) | 0.0167 (9) | 0.0074 (10) |
| C4 | 0.0415 (11) | 0.1137 (19) | 0.0455 (11) | −0.0179 (12) | 0.0106 (9) | 0.0083 (12) |
| C5 | 0.0641 (13) | 0.0781 (15) | 0.0387 (10) | −0.0288 (11) | 0.0103 (9) | −0.0025 (9) |
| C6 | 0.0539 (11) | 0.0570 (11) | 0.0318 (9) | −0.0069 (9) | 0.0146 (8) | −0.0020 (8) |
| C7 | 0.0415 (9) | 0.0381 (9) | 0.0364 (9) | −0.0001 (7) | 0.0123 (7) | −0.0007 (7) |
| C8 | 0.0578 (11) | 0.0555 (12) | 0.0491 (11) | −0.0065 (9) | 0.0245 (10) | 0.0092 (9) |
| C9 | 0.0665 (12) | 0.0551 (12) | 0.0417 (10) | −0.0017 (9) | 0.0239 (10) | 0.0093 (8) |
| C10 | 0.0748 (15) | 0.1027 (19) | 0.0776 (15) | −0.0227 (14) | 0.0402 (13) | 0.0156 (14) |
| C11 | 0.0423 (10) | 0.0619 (12) | 0.0494 (11) | −0.0140 (9) | 0.0144 (8) | −0.0084 (9) |
| C12 | 0.0401 (10) | 0.0747 (14) | 0.0485 (11) | −0.0024 (9) | 0.0127 (8) | −0.0044 (9) |
| C13 | 0.0479 (12) | 0.117 (2) | 0.0612 (13) | −0.0011 (13) | 0.0050 (10) | −0.0043 (13) |
| Cl1 | 0.0614 (3) | 0.0629 (3) | 0.0409 (3) | 0.0018 (2) | 0.0135 (2) | 0.0051 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C7 | 1.7111 (17) | C11—C12 | 1.510 (3) |
| S1—C9 | 1.723 (2) | C12—C13 | 1.517 (3) |
| O1—C12 | 1.407 (2) | C2—H2 | 0.9300 |
| O1—H1A | 0.8200 | C3—H3 | 0.9300 |
| N1—C7 | 1.333 (2) | C4—H4 | 0.9300 |
| N1—C1 | 1.424 (2) | C5—H5 | 0.9300 |
| N2—C8 | 1.409 (2) | C6—H6 | 0.9300 |
| N2—C11 | 1.468 (2) | C9—H9 | 0.9300 |
| N2—C7 | 1.341 (2) | C10—H10A | 0.9600 |
| N1—H1 | 0.8600 | C10—H10B | 0.9600 |
| C1—C2 | 1.383 (2) | C10—H10C | 0.9600 |
| C1—C6 | 1.387 (2) | C11—H11A | 0.9700 |
| C2—C3 | 1.378 (3) | C11—H11B | 0.9700 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.370 (3) | C12—H12 | 0.9800 |
| C4—C5 | 1.378 (3) | C13—H13A | 0.9600 |
| C5—C6 | 1.381 (3) | C13—H13B | 0.9600 |
| C8—C9 | 1.321 (3) | C13—H13C | 0.9600 |
| C8—C10 | 1.490 (3) | | |

| | | | |
|---|---|---|---|
| C7—S1—C9 | 90.08 (9) | C4—C3—H3 | 120.00 |
| C12—O1—H1A | 109.00 | C3—C4—H4 | 120.00 |
| C1—N1—C7 | 121.86 (14) | C5—C4—H4 | 120.00 |
| C7—N2—C11 | 123.21 (14) | C4—C5—H5 | 120.00 |
| C8—N2—C11 | 123.78 (15) | C6—C5—H5 | 120.00 |
| C7—N2—C8 | 112.74 (14) | C1—C6—H6 | 120.00 |
| C7—N1—H1 | 119.00 | C5—C6—H6 | 120.00 |
| C1—N1—H1 | 119.00 | S1—C9—H9 | 124.00 |
| N1—C1—C2 | 118.53 (15) | C8—C9—H9 | 124.00 |
| N1—C1—C6 | 120.85 (15) | C8—C10—H10A | 109.00 |
| C2—C1—C6 | 120.58 (16) | C8—C10—H10B | 110.00 |
| C1—C2—C3 | 119.24 (17) | C8—C10—H10C | 109.00 |
| C2—C3—C4 | 120.57 (19) | H10A—C10—H10B | 109.00 |
| C3—C4—C5 | 120.2 (2) | H10A—C10—H10C | 109.00 |
| C4—C5—C6 | 120.2 (2) | H10B—C10—H10C | 109.00 |
| C1—C6—C5 | 119.21 (17) | N2—C11—H11A | 109.00 |
| S1—C7—N1 | 123.50 (14) | N2—C11—H11B | 109.00 |
| S1—C7—N2 | 112.07 (12) | C12—C11—H11A | 109.00 |
| N1—C7—N2 | 124.42 (15) | C12—C11—H11B | 109.00 |
| N2—C8—C9 | 112.37 (18) | H11A—C11—H11B | 108.00 |
| N2—C8—C10 | 120.73 (16) | O1—C12—H12 | 109.00 |
| C9—C8—C10 | 126.90 (18) | C11—C12—H12 | 109.00 |
| S1—C9—C8 | 112.74 (15) | C13—C12—H12 | 109.00 |
| N2—C11—C12 | 113.11 (15) | C12—C13—H13A | 109.00 |
| O1—C12—C11 | 111.54 (16) | C12—C13—H13B | 109.00 |
| O1—C12—C13 | 108.34 (16) | C12—C13—H13C | 109.00 |
| C11—C12—C13 | 109.20 (18) | H13A—C13—H13B | 109.00 |
| C1—C2—H2 | 120.00 | H13A—C13—H13C | 109.00 |
| C3—C2—H2 | 120.00 | H13B—C13—H13C | 109.00 |
| C2—C3—H3 | 120.00 | | |

| | | | |
|---|---|---|---|
| C9—S1—C7—N1 | 178.77 (15) | C8—N2—C7—N1 | −178.65 (16) |
| C9—S1—C7—N2 | −0.17 (14) | C8—N2—C11—C12 | −94.2 (2) |
| C7—S1—C9—C8 | 0.00 (17) | N1—C1—C2—C3 | −178.13 (16) |
| C7—N1—C1—C2 | −127.80 (17) | C2—C1—C6—C5 | 0.7 (3) |
| C7—N1—C1—C6 | 54.5 (2) | N1—C1—C6—C5 | 178.37 (16) |
| C1—N1—C7—S1 | 3.0 (2) | C6—C1—C2—C3 | −0.4 (3) |
| C1—N1—C7—N2 | −178.18 (16) | C1—C2—C3—C4 | −0.2 (3) |
| C8—N2—C7—S1 | 0.27 (19) | C2—C3—C4—C5 | 0.4 (3) |
| C11—N2—C7—S1 | −173.96 (13) | C3—C4—C5—C6 | −0.1 (3) |
| C11—N2—C7—N1 | 7.1 (3) | C4—C5—C6—C1 | −0.4 (3) |
| C7—N2—C8—C9 | −0.3 (2) | N2—C8—C9—S1 | 0.1 (2) |
| C11—N2—C8—C9 | 173.93 (17) | C10—C8—C9—S1 | −178.99 (18) |

| | | | |
|---|---|---|---|
| C7—N2—C8—C10 | 178.92 (18) | N2—C11—C12—O1 | 52.9 (2) |
| C11—N2—C8—C10 | −6.9 (3) | N2—C11—C12—C13 | 172.58 (15) |
| C7—N2—C11—C12 | 79.4 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···Cl1 | 0.82 | 2.36 | 3.1681 (16) | 169 |
| N1—H1···Cl1$^{i}$ | 0.86 | 2.34 | 3.1675 (14) | 163 |
| C11—H11*A*···Cl1$^{i}$ | 0.97 | 2.81 | 3.6440 (19) | 144 |

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