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

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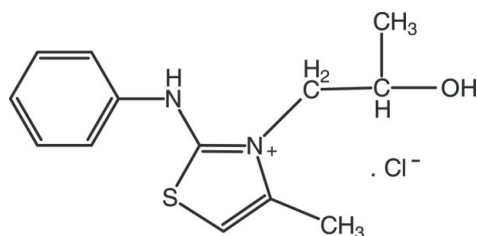
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 15.9.

In the title compound, $\text{C}_{13}\text{H}_{17}\text{N}_2\text{OS}^+\text{Cl}^-$, the thiazolium ring mean plane makes a dihedral angle of $55.46(9)^\circ$ with the benzene ring. In the propanol group, the $\text{N}-\text{C}-\text{C}$ and $\text{N}-\text{C}-\text{C}-\text{O}$ torsion angles are $172.58(15)$ and $52.9(2)^\circ$, respectively, and the $\text{S}-\text{C}-\text{C}$ torsion angle is $178.99(18)^\circ$. In the crystal, molecules are linked by $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming zigzag chains along $[001]$. There is also a $\text{C}-\text{H}\cdots\text{Cl}$ 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.* (2012a,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

| | |
|--|---------------------------------|
| $\text{C}_{13}\text{H}_{17}\text{N}_2\text{OS}^+\text{Cl}^-$ | $b = 12.2477(4)$ Å |
| $M_r = 284.81$ | $c = 10.2954(3)$ Å |
| Monoclinic, $P2_1/c$ | $\beta = 106.532(1)^\circ$ |
| $a = 11.7570(4)$ Å | $V = 1421.21(8)$ Å ³ |

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.41$ mm⁻¹

$T = 296$ K
 $0.35 \times 0.22 \times 0.20$ mm

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O1}-\text{H1A}\cdots\text{Cl1}^{\text{i}}$ | 0.82 | 2.36 | 3.1681 (16) | 169 |
| $\text{N1}-\text{H1}\cdots\text{Cl1}^{\text{i}}$ | 0.86 | 2.34 | 3.1675 (14) | 163 |
| $\text{C11}-\text{H11A}\cdots\text{Cl1}^{\text{i}}$ | 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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supporting information

Acta Cryst. (2012). E68, o1881–o1882 [doi:10.1107/S1600536812023197]

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

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S1. 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 essentially 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).

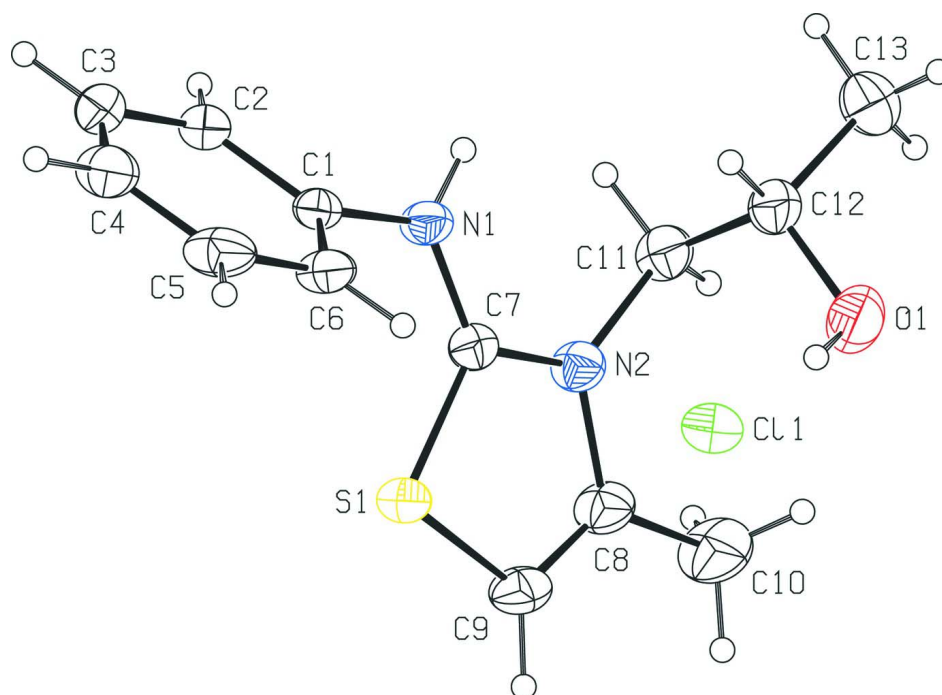
In the crystal, molecules are linked by O—H...Cl, N—H...Cl and C—H...Cl hydrogen bonds, into infinite zigzag chains propagating along the [001] direction (Table 1, Fig. 2).

S2. 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].

S3. Refinement

The H atoms were located in a difference Fourier map. In the final cycles of refinement they were included in calculated positions 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 $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl groups and $= 1.2U_{\text{eq}}(\text{C},\text{N})$ for other H atoms.

**Figure 1**

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

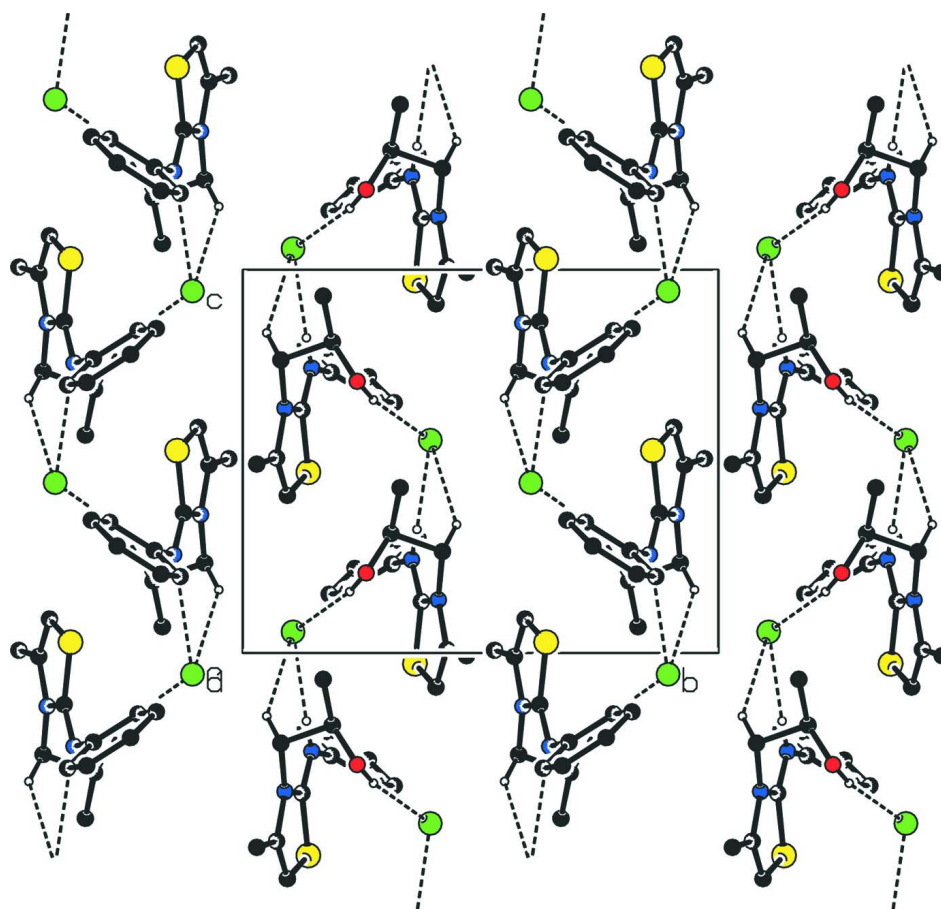


Figure 2

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: $-P\ 2_1/c$

$a = 11.7570$ (4) Å

$b = 12.2477$ (4) Å

$c = 10.2954$ (3) Å

$\beta = 106.532$ (1)°

$V = 1421.21$ (8) Å³

$Z = 4$

$F(000) = 600$

$D_x = 1.331$ 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

$0.35 \times 0.22 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0.81 pixels mm⁻¹

ω 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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 25.5^\circ$, $\theta_{\text{min}} = 2.5^\circ$
 $h = -14 \rightarrow 11$

$k = -14 \rightarrow 14$
 $l = -12 \rightarrow 12$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.18 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| 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, °)

| | | | |
|--------|-------------|----------|-----------|
| 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, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| O1—H1A...C11 | 0.82 | 2.36 | 3.1681 (16) | 169 |
| N1—H1...C11 ⁱ | 0.86 | 2.34 | 3.1675 (14) | 163 |
| C11—H11A...C11 ⁱ | 0.97 | 2.81 | 3.6440 (19) | 144 |

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