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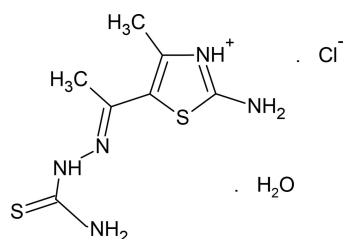
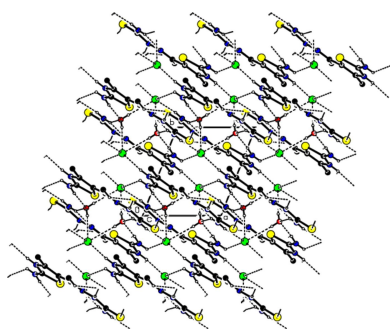
Crystal structure and Hirshfeld surface analysis of 2-amino-5-[(1*E*)-1-[(carbamothioylamino)imino]-ethyl]-4-methyl-1,3-thiazol-3-ium chloride monohydrate

Elnur Z. Huseynov,^a Mehmet Akkurt,^b Ivan Brito,^c Ajaya Bhattarai,^{d*} Farid N. Naghiyev,^a Khammed A. Asadov^a and Abel M. Maharramov^a^aDepartment of Chemistry, Baku State University, Z. Khalilov str. 23, Az, 1148 Baku, Azerbaijan, ^bDepartment of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Türkiye, ^cDepartamento de Química, Facultad de Ciencias Básicas, Universidad de Antofagasta, Avenida Angamos 601, Casilla 170, Antofagasta 1240000, Chile, and ^dDepartment of Chemistry, M.M.A.M.C (Tribhuvan University) Biratnagar, Nepal. *Correspondence e-mail: ajaya.bhattarai@mmamc.tu.edu.np

In the hydrated title salt, $C_7H_{12}N_5S_2^+ \cdot Cl^- \cdot H_2O$, the asymmetric unit comprises one 2-amino-5-[(1*E*)-1-[(carbamothioylamino)imino]ethyl]-4-methyl-1,3-thiazol-3-ium cation, one chloride anion and one water molecule of crystallization. The cation is nearly flat (r.m.s. deviation of non-H atoms is 0.0814 Å), with the largest deviation of 0.1484 (14) Å observed for one of the methyl C atoms. In the crystal, the cations are linked by O—H...Cl, N—H...Cl, N—H...O, N—H...S and C—H...S hydrogen bonds, forming a tri-periodic network. The most important contributions to the crystal packing are from H...H (35.4%), S...H/H...S (24.4%), N...H/H...N (8.7%), Cl...H/H...Cl (8.2%) and C...H/H...C (7.7%) interactions.

1. Chemical context

Heterocyclic systems account for many important organic compounds (Maharramov *et al.*, 2011*b*; Abdelhamid *et al.*, 2014). In particular, five- and six-membered heterocycles are applied in different branches of chemistry, including sustainable chemistry (Montes *et al.*, 2018), drug design and development (Khalilov *et al.*, 2021; Tas *et al.*, 2023) or material science (Yin *et al.*, 2020). The thiazole core is one of the most common five-membered heteroaromatic ring systems (Yadigarov *et al.*, 2009; Khalilov, 2021). Thiazoles have potent biological applications and represent an essential core scaffold present in many natural (thiamine, penicillin) and synthetic medicinally important compounds (Chhabria *et al.*, 2016), such as sulfazole, ritonavir, abafungin, fanetizole, meloxicam, fentiazac, nizatidine and thiamethoxam (Fig. 1). A variety of thiazole derivatives are also used as target products as well as synthetic intermediates (Maharramov *et al.*, 2011*a*; Kekeçmuhammed *et al.*, 2022).



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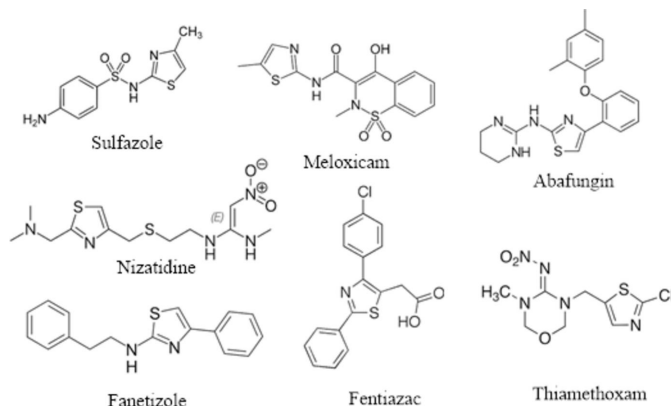


Figure 1
Chemical diagrams of some thiazole-containing marketed drugs with trade names.

In a continuation of our structural investigations of heterocyclic systems associated with biological activities (Akkurt *et al.*, 2018; Askerov *et al.*, 2020; Karimli *et al.*, 2023), we report here the crystal structure and Hirshfeld surface analysis of the hydrated title salt, $C_7H_{12}N_5S_2^+ \cdot Cl^- \cdot H_2O$, (I).

2. Structural commentary

The asymmetric unit of (I) (Fig. 2) comprises one 2-amino-5-[(1*E*)-1-[(carbamothioylamino)imino]ethyl]-4-methyl-1,3-thiazol-3-ium cation, $C_7H_{12}N_5S_2^+$, one chloride anion and one water molecule of crystallization. In the 1,3-thiazol-3-ium ring, as expected, the C1–N2 distance of 1.3309 (16) Å indicates double-bond character, while the C2–N2 distance of 1.3885 (14) Å has more single-bond character.

In the amino-*N'*-[(1*Z*)-ethylidene]ethanethiohydrazide group, the S2–C7–N4–N3, N5–C7–N4–N3, C7–N4–N3–C5 and N4–N3–C5–C6 torsion angles are 178.17 (8), –0.63 (16), 174.48 (10) and 0.16 (18)°, respectively. The title compound shows bond lengths and angles that are typical and are in agreement with those reported for the related compounds discussed in the *Database survey* section.

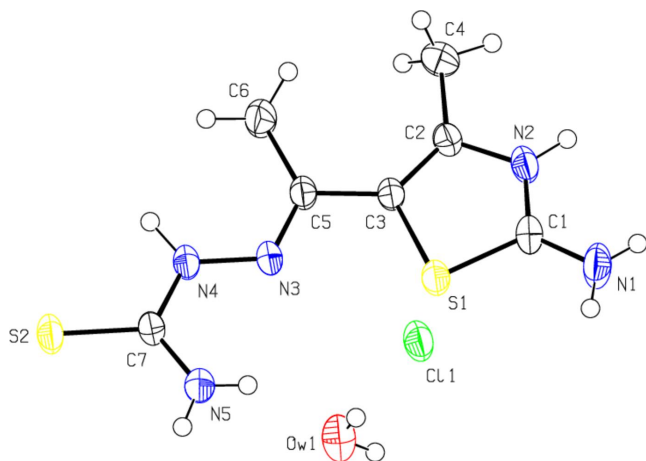


Figure 2
The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
OW1–Hw1 \cdots Cl1 ⁱ	0.79 (3)	2.45 (3)	3.2298 (13)	171 (3)
N2–H2 \cdots Cl1 ⁱⁱ	0.853 (18)	2.277 (18)	3.0812 (11)	157.2 (15)
OW1–Hw2 \cdots Cl1	0.71 (3)	2.50 (3)	3.2111 (14)	178 (3)
N1–H11 \cdots Cl1 ⁱⁱⁱ	0.78 (3)	2.81 (2)	3.2398 (15)	117.0 (18)
N1–H12 \cdots OW1 ^{iv}	0.87 (2)	1.97 (2)	2.8354 (19)	174 (2)
N4–H41 \cdots S2 ^v	0.943 (16)	2.686 (16)	3.6223 (11)	172.0 (14)
N5–H51 \cdots Cl1 ^{vi}	0.81 (2)	2.54 (2)	3.3243 (13)	164.9 (18)
N5–H52 \cdots OW1 ^{vii}	0.80 (2)	2.326 (19)	2.9899 (17)	141.2 (19)
C6–H6C \cdots S2 ^v	0.96	2.67	3.4923 (15)	143

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y, z$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, -y+2, -z$; (vi) $x-1, y+1, z$; (vii) $x, y+1, z$.

The cation is nearly flat (r.m.s. deviation of the 14 non-H atoms is 0.0814 Å), with the largest deviations observed for C6 [0.1484 (14) Å], N1 [0.1357 (10) Å], and S2 [0.1399 (6) Å].

3. Supramolecular features and Hirshfeld surface analysis

In the crystal of (I), the cations are linked by O–H \cdots Cl, N–H \cdots Cl, N–H \cdots O, N–H \cdots S and C–H \cdots S hydrogen

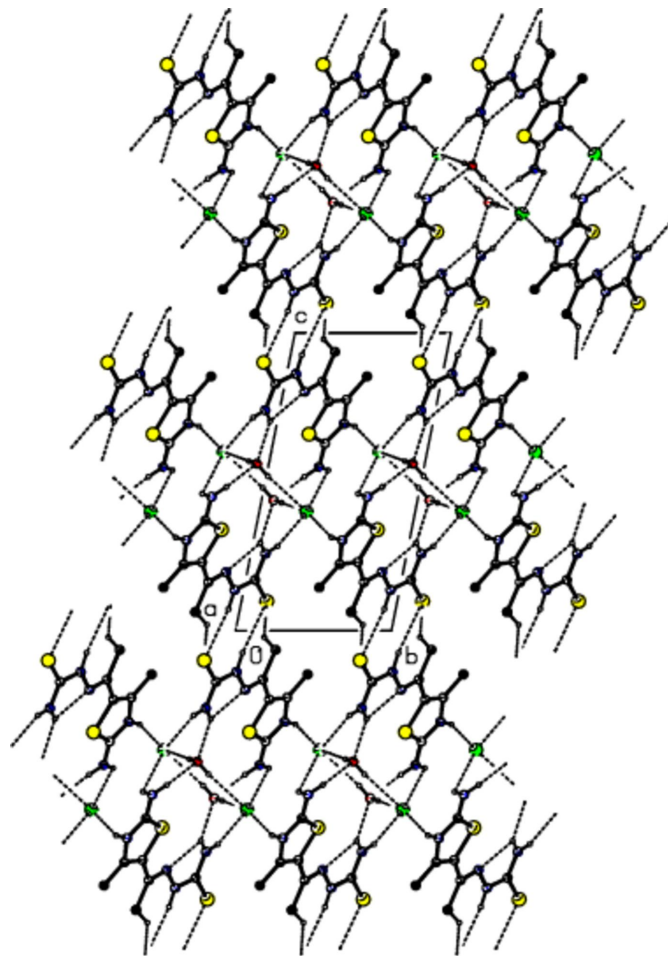


Figure 3
View of the packing of (I) along the *a* axis with the O–H \cdots Cl, N–H \cdots Cl, N–H \cdots O, N–H \cdots S and C–H \cdots S hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

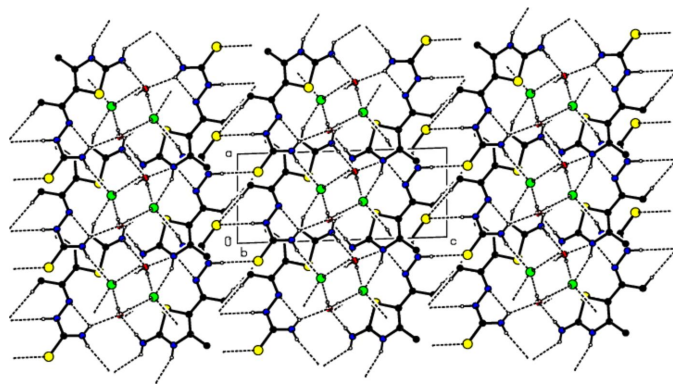


Figure 4
View of the same interactions as in Fig. 2 along the *b* axis.

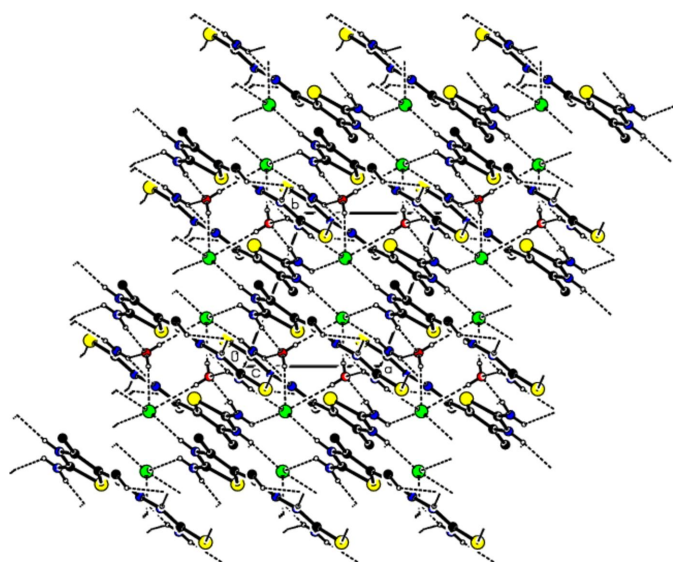


Figure 5
View of the same interactions as in Fig. 2 along the *c* axis.

bonds (Table 1), forming a tri-periodic network (Figs. 3–5). Significant C–H··· π or π – π interactions are not developed.

In order to visualize and quantify intermolecular interactions (Table 2) in (I), a Hirshfeld surface analysis was performed using *Crystal Explorer 17.5* (Spackman *et al.*, 2021), which was also used for generation of the associated two-dimensional fingerprint plots. The Hirshfeld surface mapped over d_{norm} shows the intermolecular contacts as red-colored spots, which indicate the O–H···Cl, N–H···Cl, N–H···O, N–H···S and C–H···S hydrogen bonds (Fig. 6).

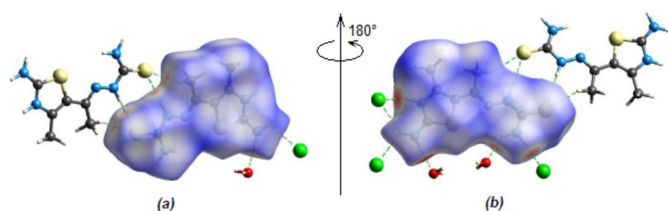


Figure 6
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of (I) mapped over d_{norm} .

Table 2
Summary of short interatomic contacts (\AA) in the title compound.

Contact	Distance	Symmetry code
H52···OW1	2.33	$x, 1 + y, z$
C1···N5	3.37	$1 + x, y, z$
C7···H4A	2.83	$-1 + x, 1 + y, z$
H6C···S2	2.67	$-x, 2 - y, -z$
H4C···S2	3.08	$1 - x, 2 - y, -z$
H2···Cl1	2.28	$1 + x, y, z$
H11···Cl1	2.81	$2 - x, 1 - y, 1 - z$
H12···OW1	1.97	$1 - x, 1 - y, 1 - z$
N1···N1	3.27	$2 - x, 1 - y, 1 - z$
H51···Cl1	2.54	$-1 + x, 1 + y, z$
C6···C4	3.55	$2 - x, 1 - y, -z$
Cl1···HW2	2.50	x, y, z
Cl1···HW1	2.45	$1 - x, -y, 1 - z$

The two-dimensional fingerprint plots of the most abundant contacts are presented in Fig. 7. H···H (35.4%) and S···H/H···S (24.4%) contacts are responsible for the largest contributions to the Hirshfeld surface. Besides these contacts,

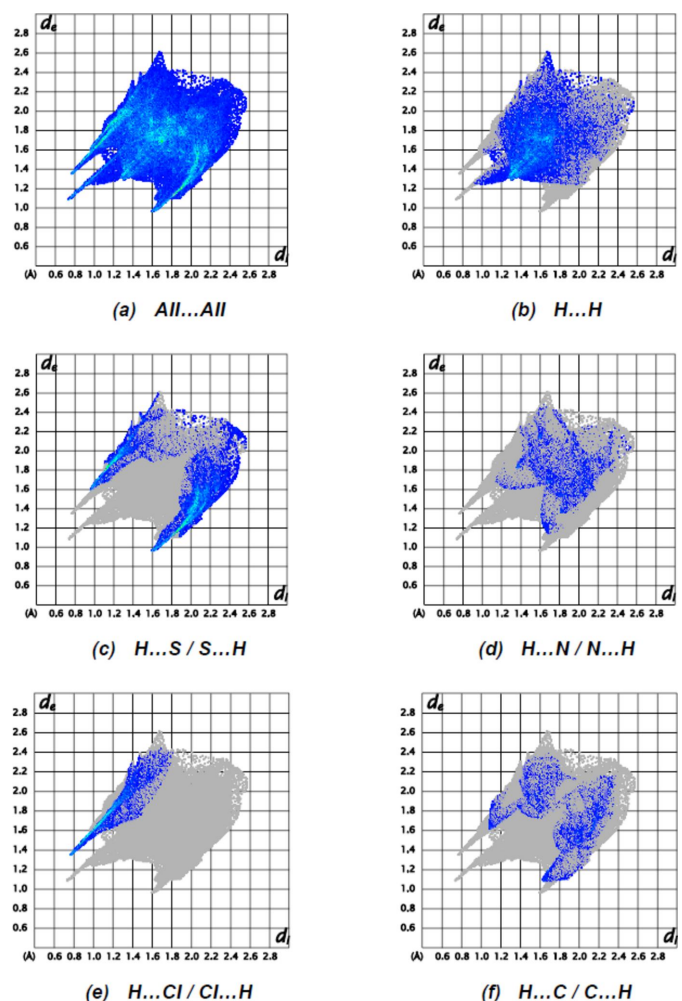


Figure 7
The two-dimensional fingerprint plots of (I), showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) S···H/H···S, (*d*) N···H/H···N, (*e*) Cl···H/H···Cl and (*f*) C···H/H···C interactions. [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

$N\cdots H/H\cdots N$ (8.7%), $Cl\cdots H/H\cdots Cl$ (8.2%) and $C\cdots H/H\cdots C$ (7.7%) interactions contribute significantly to the total Hirshfeld surface. The contributions of further contacts are only minor and amount to $C\cdots H/H\cdots C$ (4.5%), $S\cdots C/C\cdots S$ (2.4%), $N\cdots C/C\cdots N$ (2.1%), $N\cdots N$ (1.9%), $C\cdots C$ (1.6%), $S\cdots N/N\cdots S$ (1.3%), $Cl\cdots S/S\cdots Cl$ (0.6%), $Cl\cdots C/C\cdots Cl$ (0.6%), $S\cdots S$ (0.4%), $N\cdots O/O\cdots N$ (%0.1) and $S\cdots O/O\cdots S$ (0.1%).

4. Database survey

A search of the Cambridge Crystallographic Database (updated 20 March 2023; Groom *et al.*, 2016) using the 1,3-thiazol-3-ium moiety as the search fragment revealed four closely related compounds: 2-anilino-3-(2-hydroxypropyl)-4-methyl-1,3-thiazol-3-ium chloride (II) (Mohamed *et al.*, 2012), 2-amino-5-butyl-4-methyl-1,3-thiazol-3-ium nitrate (III) (Zarychta *et al.*, 2003), 2-(2-thioxo-1,3-thiazolidin-3-yl)-4,5-dihydro-1,3-thiazol-1-ium chloride (IV) (Raper *et al.*, 1996) and 2-ureido-1,3-thiazol-3-ium dihydrogen phosphate (V) (Gubina *et al.*, 2011).

In the crystal of (II), molecules are linked by $O-H\cdots Cl$ and $N-H\cdots Cl$ hydrogen bonds, forming zigzag chains along [001]. There is also a $C-H\cdots Cl$ interaction present. The crystal structure of (III) comprises a substituted thiazolium ring that is connected to a nitrate ion *via* $N-H\cdots O$ hydrogen-bonding interactions. In the crystal of (IV), the molecular packing is determined by interionic $N-H\cdots Cl$ contacts. In the crystal of (V), the molecules of substituted urea are connected by $O-H\cdots O$ hydrogen bonds into sheets. In turn, these sheets are connected to each other *via* $N-H\cdots O$ hydrogen bonds with hydrogen phosphate anions, forming a tri-periodic network.

5. Synthesis and crystallization

The title compound was synthesized using a reported procedure (Gomha *et al.*, 2016). Colorless crystals were obtained upon recrystallization from an ethanol/water (3:1 *v:v*) solution at room temperature

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms of the methyl groups were positioned geometrically and refined as riding with $C-H = 0.96 \text{ \AA}$, with $U_{iso}(H) = 1.5U_{eq}(C)$. The H atoms attached to the N atom and the H atoms of the water molecule were found in a difference-Fourier map. Their positional parameters were refined freely while setting $U_{iso}(H) = 1.2U_{eq}(N)$ and $1.5U_{eq}(O)$.

Acknowledgements

This study was supported by Baku State University, Erciyes University, Tribhuvan University and Universidad de Antofagasta. Authors' contributions are as follows. Conceptuali-

Table 3

Experimental details.

Crystal data	
Chemical formula	$C_7H_{12}N_5S_2^+Cl^- \cdot H_2O$
M_r	283.80
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	6.3279 (4), 7.7816 (6), 14.1342 (10)
α, β, γ (°)	77.191 (3), 83.660 (3), 67.860 (2)
V (Å ³)	628.35 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.62
Crystal size (mm)	0.04 × 0.03 × 0.03
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015).
T_{min}, T_{max}	0.570, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34019, 6058, 4589
R_{int}	0.053
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.833
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.036, 0.115, 1.05
No. of reflections	6058
No. of parameters	171
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.50, -0.29

Computer programs: APEX2 (Bruker, 2016), SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2020).

zation, EZH, KAA and AMM; methodology, EZH, IB and MA; investigation, EZH and IB; writing (original draft), MA and AB; writing (review and editing of the manuscript), MA and EZH; visualization, MA, FNN and IB; funding acquisition, EZH, AB and IB; resources, AB, IB and MA; supervision, MA and AMM

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supporting information

Acta Cryst. (2023). E79, 808-812 [https://doi.org/10.1107/S2056989023007090]

Crystal structure and Hirshfeld surface analysis of 2-amino-5- $\{$ (1*E*)-1-[(carbamothioylamino)imino]ethyl $\}$ -4-methyl-1,3-thiazol-3-ium chloride monohydrate

Elnur Z. Huseynov, Mehmet Akkurt, Ivan Brito, Ajaya Bhattarai, Farid N. Naghiyev, Khammed A. Asadov and Abel M. Maharramov

Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

2-Amino-5- $\{$ (1*E*)-1-[(carbamothioylamino)imino]ethyl $\}$ -4-methyl-1,3-thiazol-3-ium chloride monohydrate

Crystal data

$C_7H_{12}N_5S_2^+ \cdot Cl^- \cdot H_2O$

$M_r = 283.80$

Triclinic, $P\bar{1}$

$a = 6.3279$ (4) Å

$b = 7.7816$ (6) Å

$c = 14.1342$ (10) Å

$\alpha = 77.191$ (3)°

$\beta = 83.660$ (3)°

$\gamma = 67.860$ (2)°

$V = 628.35$ (8) Å³

$Z = 2$

$F(000) = 296$

$D_x = 1.500$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9921 reflections

$\theta = 3.0$ – 36.3 °

$\mu = 0.62$ mm⁻¹

$T = 293$ K

Prism, colourless

$0.04 \times 0.03 \times 0.03$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015).

$T_{\min} = 0.570$, $T_{\max} = 0.747$

34019 measured reflections

6058 independent reflections

4589 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.053$

$\theta_{\max} = 36.3$ °, $\theta_{\min} = 3.0$ °

$h = -10 \rightarrow 10$

$k = -12 \rightarrow 12$

$l = -23 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.115$

$S = 1.05$

6058 reflections

171 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.0995P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.50$ e Å⁻³

$\Delta\rho_{\min} = -0.29$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.00052 (18)	0.66580 (16)	0.37114 (8)	0.0336 (2)
C2	1.00425 (17)	0.58328 (15)	0.22387 (8)	0.03023 (18)
C3	0.78120 (16)	0.69558 (14)	0.23070 (7)	0.02811 (17)
C4	1.1391 (2)	0.4821 (2)	0.14588 (10)	0.0429 (3)
H4A	1.053893	0.420248	0.123677	0.064*
H4B	1.281001	0.389685	0.171192	0.064*
H4C	1.169126	0.571545	0.092670	0.064*
C5	0.59592 (16)	0.76248 (15)	0.16319 (7)	0.02893 (17)
C6	0.6438 (2)	0.7189 (2)	0.06335 (10)	0.0474 (3)
H6A	0.648883	0.593175	0.065682	0.071*
H6B	0.788013	0.727617	0.039126	0.071*
H6C	0.525339	0.807944	0.021177	0.071*
C7	0.01732 (16)	1.05991 (15)	0.17123 (7)	0.02918 (17)
N1	1.0867 (2)	0.6736 (2)	0.45014 (10)	0.0471 (3)
H11	1.215 (4)	0.611 (3)	0.4604 (14)	0.057*
H12	0.992 (4)	0.756 (3)	0.4827 (15)	0.057*
N2	1.12182 (15)	0.56820 (14)	0.30449 (7)	0.03419 (18)
H2	1.261 (3)	0.496 (2)	0.3136 (12)	0.041*
N3	0.40159 (14)	0.86322 (14)	0.19705 (7)	0.03073 (16)
N4	0.21575 (15)	0.94127 (14)	0.13782 (7)	0.03273 (18)
H41	0.214 (3)	0.927 (2)	0.0734 (12)	0.039*
N5	0.01285 (18)	1.09259 (17)	0.25930 (8)	0.0395 (2)
H51	-0.101 (3)	1.160 (3)	0.2836 (13)	0.047*
H52	0.117 (3)	1.046 (3)	0.2953 (13)	0.047*
S1	0.71982 (4)	0.78020 (4)	0.33975 (2)	0.03514 (7)
S2	-0.21036 (5)	1.16255 (5)	0.09918 (2)	0.03939 (8)
Cl1	0.57747 (5)	0.30475 (5)	0.39936 (2)	0.04264 (8)
OW1	0.23501 (19)	0.07771 (18)	0.43851 (9)	0.0517 (3)
HW1	0.288 (4)	-0.009 (4)	0.4806 (19)	0.078*
HW2	0.308 (4)	0.131 (4)	0.4302 (19)	0.078*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0290 (4)	0.0352 (5)	0.0351 (5)	-0.0092 (4)	-0.0118 (4)	-0.0030 (4)
C2	0.0241 (4)	0.0307 (4)	0.0325 (4)	-0.0064 (3)	-0.0040 (3)	-0.0042 (3)
C3	0.0230 (4)	0.0313 (4)	0.0283 (4)	-0.0065 (3)	-0.0052 (3)	-0.0062 (3)
C4	0.0341 (5)	0.0456 (6)	0.0429 (6)	-0.0052 (5)	0.0031 (4)	-0.0152 (5)
C5	0.0240 (4)	0.0324 (4)	0.0296 (4)	-0.0081 (3)	-0.0065 (3)	-0.0057 (3)

C6	0.0341 (5)	0.0638 (8)	0.0390 (6)	-0.0028 (5)	-0.0082 (4)	-0.0231 (6)
C7	0.0230 (4)	0.0327 (4)	0.0301 (4)	-0.0080 (3)	-0.0063 (3)	-0.0037 (3)
N1	0.0405 (5)	0.0552 (7)	0.0440 (6)	-0.0094 (5)	-0.0204 (4)	-0.0116 (5)
N2	0.0236 (3)	0.0361 (4)	0.0378 (4)	-0.0047 (3)	-0.0092 (3)	-0.0043 (3)
N3	0.0225 (3)	0.0370 (4)	0.0303 (4)	-0.0071 (3)	-0.0071 (3)	-0.0054 (3)
N4	0.0236 (3)	0.0403 (5)	0.0309 (4)	-0.0050 (3)	-0.0076 (3)	-0.0086 (3)
N5	0.0290 (4)	0.0525 (6)	0.0316 (4)	-0.0055 (4)	-0.0053 (3)	-0.0121 (4)
S1	0.02593 (11)	0.04268 (15)	0.03359 (13)	-0.00389 (10)	-0.00727 (9)	-0.01324 (11)
S2	0.02756 (12)	0.04546 (16)	0.03856 (14)	-0.00214 (10)	-0.01341 (10)	-0.00894 (12)
Cl1	0.02891 (12)	0.04757 (16)	0.04456 (16)	-0.00184 (10)	-0.01143 (10)	-0.01183 (12)
OW1	0.0426 (5)	0.0549 (6)	0.0542 (6)	-0.0121 (4)	-0.0169 (4)	-0.0060 (5)

Geometric parameters (Å, °)

C1—N1	1.3181 (16)	C6—H6B	0.9600
C1—N2	1.3309 (16)	C6—H6C	0.9600
C1—S1	1.7180 (11)	C7—N5	1.3198 (15)
C2—C3	1.3575 (13)	C7—N4	1.3567 (14)
C2—N2	1.3885 (14)	C7—S2	1.6872 (10)
C2—C4	1.4945 (16)	N1—H11	0.79 (2)
C3—C5	1.4570 (14)	N1—H12	0.87 (2)
C3—S1	1.7565 (10)	N2—H2	0.854 (18)
C4—H4A	0.9600	N3—N4	1.3806 (12)
C4—H4B	0.9600	N4—H41	0.943 (17)
C4—H4C	0.9600	N5—H51	0.81 (2)
C5—N3	1.2906 (13)	N5—H52	0.80 (2)
C5—C6	1.4961 (16)	OW1—HW1	0.78 (3)
C6—H6A	0.9600	OW1—HW2	0.71 (3)
N1—C1—N2	124.00 (11)	C5—C6—H6C	109.5
N1—C1—S1	124.99 (10)	H6A—C6—H6C	109.5
N2—C1—S1	111.01 (8)	H6B—C6—H6C	109.5
C3—C2—N2	111.36 (9)	N5—C7—N4	117.81 (9)
C3—C2—C4	131.66 (10)	N5—C7—S2	122.67 (8)
N2—C2—C4	116.95 (9)	N4—C7—S2	119.51 (8)
C2—C3—C5	131.75 (10)	C1—N1—H11	118.0 (15)
C2—C3—S1	111.21 (8)	C1—N1—H12	113.9 (14)
C5—C3—S1	116.95 (7)	H11—N1—H12	127.9 (19)
C2—C4—H4A	109.5	C1—N2—C2	115.94 (9)
C2—C4—H4B	109.5	C1—N2—H2	120.9 (11)
H4A—C4—H4B	109.5	C2—N2—H2	123.1 (11)
C2—C4—H4C	109.5	C5—N3—N4	118.97 (9)
H4A—C4—H4C	109.5	C7—N4—N3	118.45 (9)
H4B—C4—H4C	109.5	C7—N4—H41	115.1 (10)
N3—C5—C3	113.92 (9)	N3—N4—H41	126.3 (10)
N3—C5—C6	126.22 (10)	C7—N5—H51	122.4 (14)
C3—C5—C6	119.81 (9)	C7—N5—H52	125.2 (13)
C5—C6—H6A	109.5	H51—N5—H52	112.4 (18)

C5—C6—H6B	109.5	C1—S1—C3	90.43 (5)
H6A—C6—H6B	109.5	HW1—OW1—HW2	106 (3)
N2—C2—C3—C5	175.76 (11)	C4—C2—N2—C1	177.27 (11)
C4—C2—C3—C5	-2.4 (2)	C3—C5—N3—N4	177.15 (9)
N2—C2—C3—S1	-0.57 (12)	C6—C5—N3—N4	-0.16 (18)
C4—C2—C3—S1	-178.69 (11)	N5—C7—N4—N3	-0.63 (16)
C2—C3—C5—N3	177.59 (11)	S2—C7—N4—N3	178.17 (8)
S1—C3—C5—N3	-6.25 (13)	C5—N3—N4—C7	-174.48 (10)
C2—C3—C5—C6	-4.92 (19)	N1—C1—S1—C3	177.38 (12)
S1—C3—C5—C6	171.25 (10)	N2—C1—S1—C3	-2.17 (9)
N1—C1—N2—C2	-177.21 (12)	C2—C3—S1—C1	1.55 (9)
S1—C1—N2—C2	2.34 (13)	C5—C3—S1—C1	-175.38 (9)
C3—C2—N2—C1	-1.15 (14)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
OW1—HW1 \cdots C11 ⁱ	0.79 (3)	2.45 (3)	3.2298 (13)	171 (3)
N2—H2 \cdots C11 ⁱⁱ	0.853 (18)	2.277 (18)	3.0812 (11)	157.2 (15)
OW1—HW2 \cdots C11	0.71 (3)	2.50 (3)	3.2111 (14)	178 (3)
N1—H11 \cdots C11 ⁱⁱⁱ	0.78 (3)	2.81 (2)	3.2398 (15)	117.0 (18)
N1—H12 \cdots OW1 ^{iv}	0.87 (2)	1.97 (2)	2.8354 (19)	174 (2)
N4—H41 \cdots S2 ^v	0.943 (16)	2.686 (16)	3.6223 (11)	172.0 (14)
N5—H51 \cdots C11 ^{vi}	0.81 (2)	2.54 (2)	3.3243 (13)	164.9 (18)
N5—H52 \cdots OW1 ^{vii}	0.80 (2)	2.326 (19)	2.9899 (17)	141.2 (19)
N5—H52 \cdots N3	0.80 (2)	2.36 (2)	2.6306 (16)	100.6 (15)
C6—H6C \cdots N4	0.96	2.48	2.8433 (18)	102
C6—H6C \cdots S2 ^v	0.96	2.67	3.4923 (15)	143

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y, z$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, -y+2, -z$; (vi) $x-1, y+1, z$; (vii) $x, y+1, z$.