research communications

Crystal structure and Hirshfeld surface analysis of 1-(2-amino-4-methyl-1,3-thiazol-5-yl)ethan-1-one

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In the title compound, $C_6H_8N_2OS$, all atoms except for the methyl H atoms are coplanar, with a maximum deviation of 0.026 (4) Å. In the crystal, pairs of molecules are linked by N—H···N hydrogen bonds, forming $R_2^2(8)$ ring motifs. Dimers are connected by N—H···O hydrogen bonds, forming layers parallel to the (102) plane. Consolidating the molecular packing, these layers are connected by C—H···π interactions between the center of the 1,3-thiazole ring and the H atom of the methyl group attached to it, as well as C=O···π interactions between the center of the 1,3-thiazole ring and the O atom of the carboxyl group. According to a Hirshfeld surface study, H···H (37.6%), O···H/H···O (16.8%), S···H/H···S (15.4%), N···H/H···N (13.0%) and C···H/H···C (7.6%) interactions are the most significant contributors to the crystal packing.

1. Chemical context

Heterocyclic aromatic systems are the most important and manifold compounds in organic chemistry (Maharramov *et al.*, 2011*b*; Abdelhamid *et al.*, 2014). Organic synthesis is developing intensely with newer aromatic heterocyclic compounds that are obtained for diverse medicinal and commercial purposes (Khalilov *et al.*, 2021). Nowadays, applications of five- and six-membered ring heterocycles have expanded in different branches of chemistry, including sustainable chem-
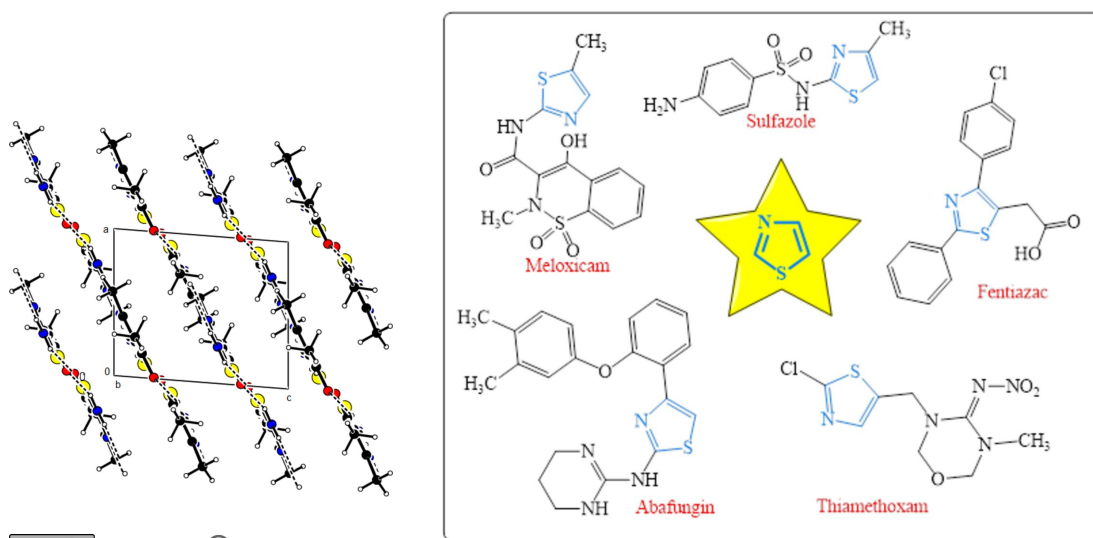

Figure 1
Some marketed drugs containing the thiazole moiety.

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

$Cg1$ is the centroid of the (N1/S1/C1–C3) 1,3-thiazole ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H1$A\cdots$N1^i	0.86	2.11	2.963 (4)	175
N2—H1$B\cdots$O1^{ii}	0.86	2.02	2.835 (4)	158
C4—H4$B\cdots Cg1^{iii}$	0.96	2.89	3.603 (4)	132

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

istry (Montes *et al.*, 2018), drug design and development (Tas *et al.*, 2023) and materials sciences (Yin *et al.*, 2020). The thiazole core is the most common five-membered heteroaromatic ring system in azole heterocycles (Yadigarov *et al.*, 2009; Khalilov, 2021). Thiazoles have potent medicinal applications as it is 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, thiamethoxam, *etc.* (Fig. 1). On the other hand, there have been a variety of significant examples of thiazole derivatives used as target products as well as synthetic intermediates (Akkurt *et al.*, 2018; Kekeçmuhammed *et al.*, 2022).
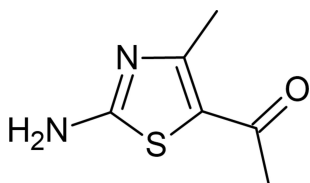
In a continuation of our investigations of heterocyclic systems with biological activity and in the framework of ongoing structural studies (Maharramov *et al.*, 2011*a*; Askerov *et al.*, 2020; Karimli *et al.*, 2023), we report here the crystal structure and Hirshfeld surface analysis of the title compound, 1-(2-amino-4-methyl-1,3-thiazol-5-yl)ethan-1-one.
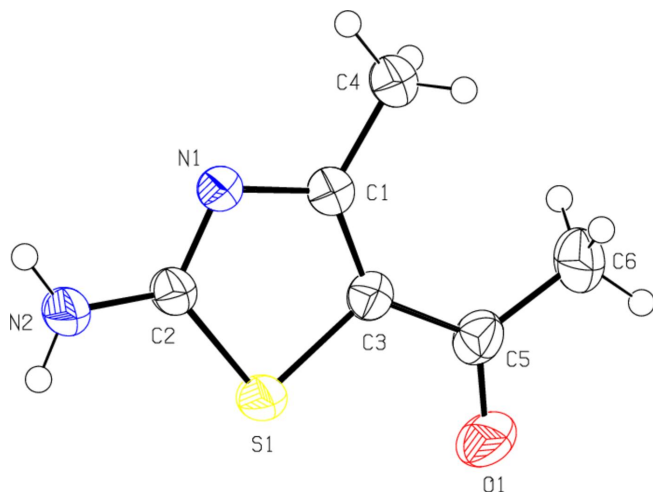
Figure 2
The molecular structure of the title compound, showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.
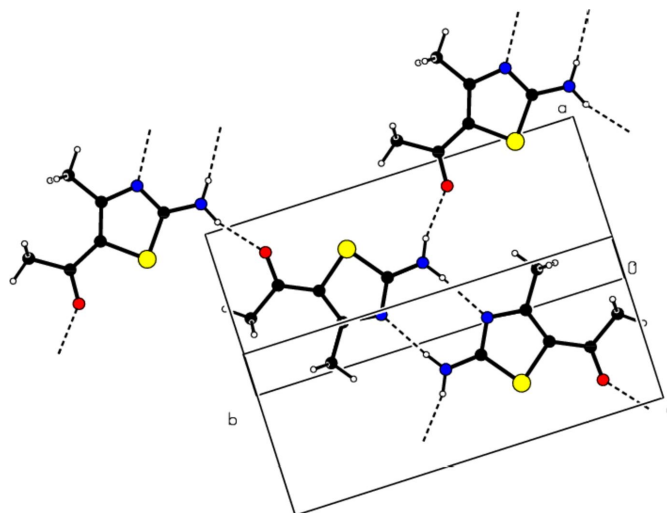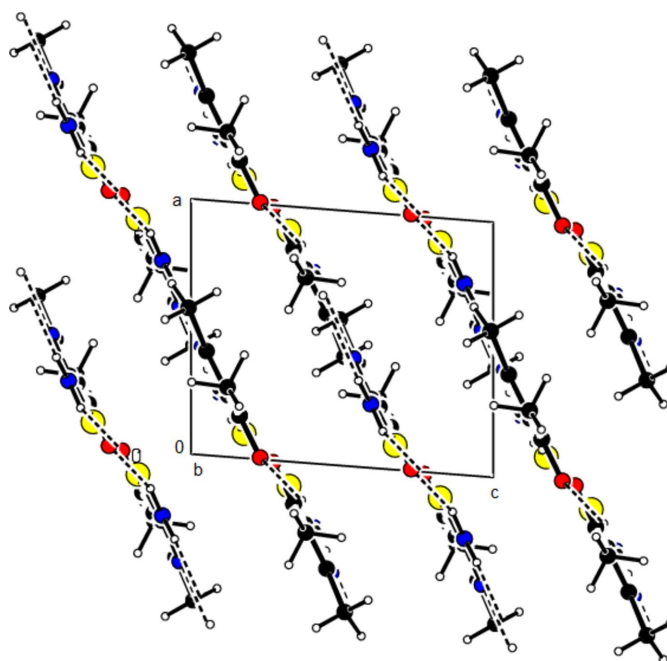
Figure 3
Partial view of the N—H$\cdots$N and N—H$\cdots$O bonds in the (102) plane of the title compound.

2. Structural commentary

In the title compound, Fig. 2, all atoms except for the methyl H atoms are coplanar, with a maximum deviation of 0.026 (4) Å for C6. The geometric parameters of the title compound are normal and comparable to those of related compounds listed in the *Database survey* section.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, pairs of molecules are linked by N—H$\cdots$N hydrogen bonds, forming $R_2^2(8)$ ring motifs (Bernstein *et al.*,

Figure 4
View of the packing of the title compound along the *b*-axis.

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

O1···H4A	2.69	$1 + x, y, z$
O1···H1B	2.02	$2 - x, \frac{1}{2} + y, \frac{1}{2} - z$
C1···H4B	3.09	$x, \frac{3}{2} - y, -\frac{1}{2} + z$
H1A···N1	2.11	$1 - x, 1 - y, 1 - z$
N2···H6B	2.89	$1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$

1995; Table 1, Fig. 3). Dimers are connected by N—H···O hydrogen bonds, forming layers parallel to the (102) plane (Table 1, Fig. 4). Consolidating the molecular packing, these layers are connected by C—H···π interactions between the center of the 1,3-thiazole ring and the H atom of the methyl group attached to it, as well as C=O···π interactions between the center of the 1,3-thiazole ring and the O atom of the carboxyl group (Table 1, Figs. 5 and 6).
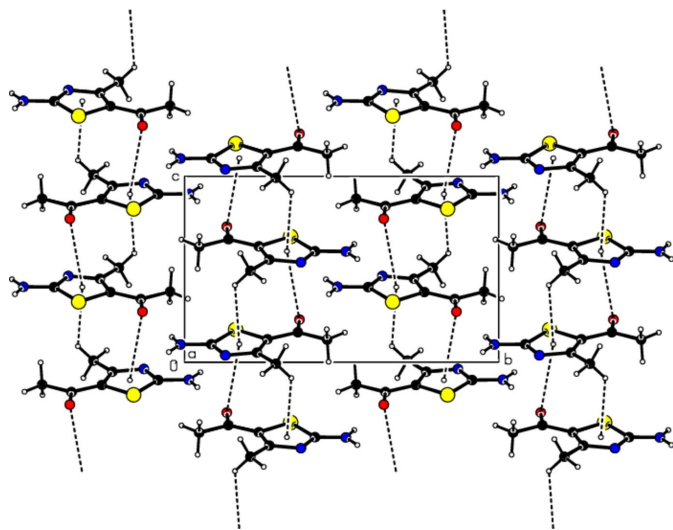

Figure 7
(a) Front and (b) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}, with a fixed color scale of -0.5624 to 0.9850 a.u.

Crystal Explorer 17.5 (Spackman *et al.*, 2021) was used to generate Hirshfeld surfaces and two-dimensional fingerprint plots in order to quantify the intermolecular interactions in

Figure 5
View of the C—H···π and C=O···π interactions of the title compound down the *a* axis.
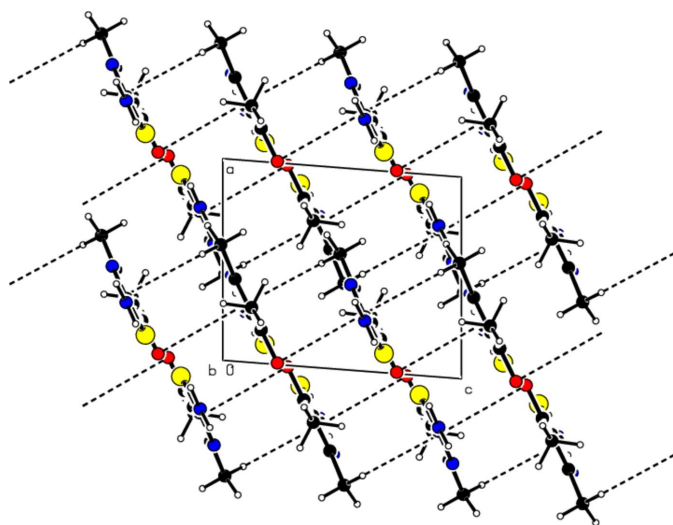
Figure 6
View of the C—H···π and C=O···π interactions of the title compound down the *b* axis.

Figure 8
The two-dimensional fingerprint plots of the title compound, showing (a) all interactions, and delineated into (b) H···H, (c) O···H/H···O, (d) S···H/H···S, (e) N···H/H···N 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].

the crystal. The Hirshfeld surfaces were mapped over d_{norm} in the range -0.5624 (red) to 0.9850 (blue) a.u. (Fig. 7). The interactions giv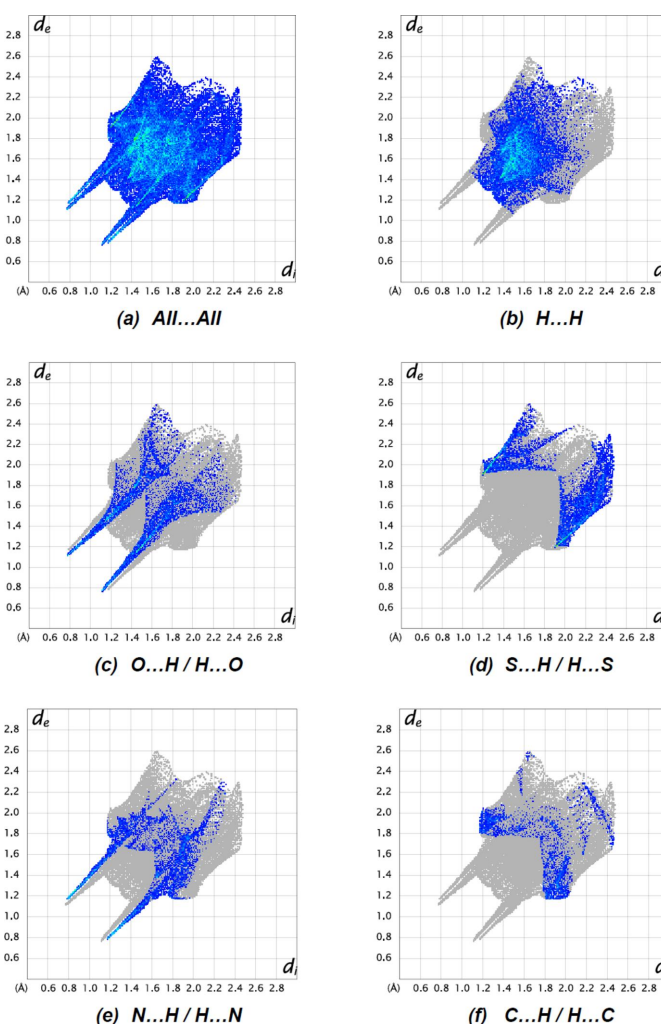en in Table 2 play a key role in the molecular packing of the title compound. The most important interatomic contact is $H \cdots H$ as it makes the highest contribution to the crystal packing (37.6%, Fig. 8b). Other major contributors are $O \cdots H/H \cdots O$ (16.8%, Fig. 8c), $S \cdots H/H \cdots S$ (15.4%, Fig. 8d), $N \cdots H/H \cdots N$ (13.0%, Fig. 8e) and $C \cdots H/H \cdots C$ (7.6%, Fig. 8f) interactions. Other, smaller contributions are made by $S \cdots C/C \cdots S$ (2.7%), $C \cdots O/O \cdots C$ (2.6%), $C \cdots C$ (1.8%), $N \cdots C/C \cdots N$ (1.5%), $S \cdots O/O \cdots S$ (0.8%), $S \cdots N/ N \cdots S$ (0.1%) and $O \cdots N/N \cdots O$ (0.1%) interactions.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update November 2022; Groom *et al.*, 2016) for the central five-membered ring *1,3-thiazole* yielded five compounds related to the title compound, *viz.* CSD refcodes IXAMAV (Kennedy *et al.*, 2004a), ABEGAQ (Kennedy *et al.*, 2004b), FEFKUY (Hazra *et al.*, 2012), DUTZEY (Chen & Xu, 2010) and LAMQOJ (Fait *et al.*, 2021).

In the crystal of IXAMAV, the supramolecular network is based upon $N-H \cdots N$ hydrogen-bonded centrosymmetric dimers linked by $N-H \cdots O$ contacts. ABEGAQ forms a supramolecular network based on $N-H \cdots N$ hydrogen-bonded centrosymmetric dimers that are linked in turn by $N-H \cdots O$ contacts. In the crystal of FEFKUY, an interplay of $O-H \cdots N$ and $C-H \cdots O$ hydrogen bonds connects the molecules to form $C(6)R_2^2(8)$ polymeric chains, which are further linked *via* weak $C-H \cdots O$ hydrogen bonds into a two-dimensional supramolecular framework. The crystal structure of DUTZEY involves intermolecular $N-H \cdots N$ hydrogen bonds. In the crystal of LAMQOJ, weak $C-H \cdots N$ hydrogen bonds build up a wavy layer of molecules in the (011) plane. The layers are stacked in the [100] direction by weak $\pi-\pi$ stacking interactions between the 1,3-thiazole rings.

5. Synthesis and crystallization

The title compound was synthesized using a reported procedure (Donald *et al.*, 2012), and colorless crystals were obtained upon recrystallization from an ethanol/water (3:1) solution at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were placed in calculated positions ($C-H = 0.96$ Å and $N-H = 0.86$ Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(N)$ for the NH_2 group and $1.5U_{eq}(C)$ for CH_3 groups.

Acknowledgements

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Table 3
Experimental details.

Crystal data	
Chemical formula	$C_6H_8N_2OS$
M_r	156.20
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	6.7445 (15), 13.498 (3), 8.010 (2)
β (°)	94.421 (7)
V (Å^3)	727.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.37
Crystal size (mm)	$0.60 \times 0.45 \times 0.35$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.649, 0.745
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	14701, 1492, 940
R_{int}	0.144
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.142, 1.04
No. of reflections	1492
No. of parameters	93
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.29, −0.28

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

References

Abdelhamid, A. A., Mohamed, S. K., Maharramov, A. M., Khalilov, A. N. & Allahverdiev, M. A. (2014). *J. Saudi Chem. Soc.* **18**, 474–478.

Akkurt, M., Duruskari, G. S., Toze, F. A. A., Khalilov, A. N. & Huseynova, A. T. (2018). *Acta Cryst.* E**74**, 1168–1172.

Askerov, R. K., Maharramov, A. M., Khalilov, A. N., Akkurt, M., Akobirshoeva, A. A., Osmanov, V. K. & Borisov, A. V. (2020). *Acta Cryst.* E**76**, 1007–1011.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2016). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin. USA.

Chen, X. & Xu, L. (2010). *Acta Cryst.* E**66**, o2148.

Chhabria, M. T., Patel, S., Modi, P. & Brahmkshatriya, P. S. (2016). *Curr. Top. Med. Chem.* **16**, 2841–2862.

Donald, M. B., Rodriguez, K. X., Shay, H., Phuan, P.-W., Verkman, A. S. & Kurth, M. J. (2012). *Bioorg. Med. Chem.* **20**, 5247–5253.

Fait, M. J. G., Spannenberg, A., Kondratenko, E. V. & Linke, D. (2021). *IUCrData*, **6**, x211332.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

research communications

Hazra, D. K., Mukherjee, M., Helliwell, M. & Mukherjee, A. K. (2012). *Acta Cryst.* C**68**, o452–o455.

Karimli, E. G., Khrustalev, V. N., Kurasova, M. N., Akkurt, M., Khalilov, A. N., Bhattarai, A. & Mamedov, İ. G. (2023). *Acta Cryst.* E**79**, 474–477.

Kekeçmuhammed, H., Tapera, M., Tüzün, B., Akkoç, S., Zorlu, Y. & Sarıpınar, E. (2022). *ChemistrySelect*, **7**, e202201502.

Kennedy, A. R., Khalaf, A. I., Suckling, C. J. & Waigh, R. D. (2004a). *Acta Cryst.* E**60**, o1188–o1190.

Kennedy, A. R., Khalaf, A. I., Suckling, C. J. & Waigh, R. D. (2004b). *Acta Cryst.* E**60**, o1510–o1512.

Khalilov, A. N. (2021). *Rev. Roum. Chim.* **66**, 719–723.

Khalilov, A. N., Tüzün, B., Taslimi, P., Tas, A., Tuncbilek, Z. & Cakmak, N. K. (2021). *J. Mol. Liq.* **344**, 117761.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Maharramov, A. M., Khalilov, A. N., Gurbanov, A. V., Allahverdiyev, M. A. & Ng, S. W. (2011a). *Acta Cryst.* E**67**, o721.

Maharramov, A. M., Khalilov, A. N., Gurbanov, A. V. & Brito, I. (2011b). *Acta Cryst.* E**67**, o1307.

Montes, V., Miñambres, J. F., Khalilov, A. N., Boutonnet, M., Marinas, J. M., Urbano, F. J., Maharramov, A. M. & Marinas, A. (2018). *Catal. Today*, **306**, 89–95.

Sheldrick, G. M. (2015a). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015b). *Acta Cryst.* C**71**, 3–8.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Tas, A., Tüzün, B., Khalilov, A. N., Taslimi, P., Ağbektas, T. & Cakmak, N. K. (2023). *J. Mol. Struct.* **1273**, 134282.

Yadigarov, R. R., Khalilov, A. N., Mamedov, I. G., Nagiev, F. N., Magerramov, A. M. & Allakhverdiev, M. A. (2009). *Russ. J. Org. Chem.* **45**, 1856–1858.

Yin, J., Khalilov, A. N., Muthupandi, P., Ladd, R. & Birman, V. B. (2020). *J. Am. Chem. Soc.* **142**, 60–63.

Crystal structure and Hirshfeld surface analysis of 1-(2-amino-4-methyl-1,3-thiazol-5-yl)ethan-1-one

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Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* V8.40B (Bruker, 2016); data reduction: *SAINT* V8.40B (Bruker, 2016); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

1-(2-Amino-4-methyl-1,3-thiazol-5-yl)ethan-1-one

Crystal data

$C_6H_8N_2OS$	$F(000) = 328$
$M_r = 156.20$	$D_x = 1.427$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.7445$ (15) Å	Cell parameters from 2051 reflections
$b = 13.498$ (3) Å	$\theta = 3.0–26.4°$
$c = 8.010$ (2) Å	$\mu = 0.37$ mm^{-1}
$\beta = 94.421$ (7)°	$T = 296$ K
$V = 727.1$ (3) Å^3	Prism, colourless
$Z = 4$	$0.60 \times 0.45 \times 0.35$ mm

Data collection

Bruker APEXII CCD diffractometer	1492 independent reflections
φ and ω scans	940 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015	$R_{int} = 0.144$
$T_{min} = 0.649$, $T_{max} = 0.745$	$\theta_{max} = 26.4°$, $\theta_{min} = 3.0°$
14701 measured reflections	$h = -8\rightarrow8$
	$k = -16\rightarrow16$
	$l = -10\rightarrow10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.4474P]$
$wR(F^2) = 0.142$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
1492 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
93 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
0 restraints	

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5920 (5)	0.7303 (2)	0.4486 (4)	0.0354 (8)
C2	0.7302 (5)	0.5848 (2)	0.4036 (4)	0.0356 (8)
C3	0.7583 (5)	0.7636 (2)	0.3769 (4)	0.0349 (8)
C4	0.4274 (5)	0.7905 (3)	0.5084 (5)	0.0446 (9)
H4A	0.356539	0.822440	0.414759	0.067*
H4B	0.480953	0.839710	0.585759	0.067*
H4C	0.338231	0.748209	0.563299	0.067*
C5	0.8348 (5)	0.8605 (3)	0.3393 (4)	0.0408 (9)
C6	0.7269 (6)	0.9538 (3)	0.3790 (5)	0.0567 (11)
H6A	0.718170	0.958584	0.497742	0.085*
H6B	0.595477	0.952624	0.323674	0.085*
H6C	0.798079	1.010036	0.340806	0.085*
N1	0.5761 (4)	0.62959 (19)	0.4631 (4)	0.0359 (7)
N2	0.7505 (4)	0.4865 (2)	0.4051 (4)	0.0498 (9)
H1A	0.661573	0.449933	0.445684	0.060*
H1B	0.852593	0.459698	0.365376	0.060*
S1	0.90402 (13)	0.66254 (6)	0.32437 (12)	0.0412 (3)
O1	0.9925 (4)	0.8657 (2)	0.2713 (4)	0.0571 (8)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0349 (18)	0.0323 (17)	0.039 (2)	0.0005 (15)	0.0045 (15)	−0.0011 (15)
C2	0.0348 (18)	0.0287 (16)	0.044 (2)	0.0034 (14)	0.0063 (15)	0.0031 (15)
C3	0.0343 (18)	0.0308 (17)	0.040 (2)	−0.0023 (14)	0.0035 (15)	0.0009 (15)
C4	0.042 (2)	0.0320 (18)	0.061 (2)	0.0032 (16)	0.0105 (18)	−0.0005 (17)
C5	0.0410 (19)	0.0351 (19)	0.046 (2)	−0.0044 (15)	0.0016 (17)	0.0066 (15)
C6	0.066 (3)	0.0313 (19)	0.075 (3)	0.0012 (19)	0.015 (2)	0.0054 (19)
N1	0.0318 (14)	0.0294 (14)	0.0476 (18)	−0.0007 (11)	0.0093 (13)	0.0001 (13)
N2	0.0450 (18)	0.0295 (16)	0.078 (2)	0.0006 (13)	0.0263 (17)	0.0004 (15)
S1	0.0371 (5)	0.0341 (5)	0.0547 (6)	0.0002 (4)	0.0172 (4)	0.0035 (4)
O1	0.0474 (16)	0.0460 (16)	0.080 (2)	−0.0083 (12)	0.0182 (15)	0.0148 (14)

Geometric parameters (Å, º)

C1—N1	1.370 (4)	C4—H4B	0.9600
C1—C3	1.375 (4)	C4—H4C	0.9600
C1—C4	1.484 (5)	C5—O1	1.234 (4)
C2—N1	1.322 (4)	C5—C6	1.501 (5)

C2—N2	1.334 (4)	C6—H6A	0.9600
C2—S1	1.730 (3)	C6—H6B	0.9600
C3—C5	1.446 (5)	C6—H6C	0.9600
C3—S1	1.752 (3)	N2—H1A	0.8600
C4—H4A	0.9600	N2—H1B	0.8600
N1—C1—C3	115.6 (3)	O1—C5—C3	118.5 (3)
N1—C1—C4	116.8 (3)	O1—C5—C6	119.6 (3)
C3—C1—C4	127.6 (3)	C3—C5—C6	121.9 (3)
N1—C2—N2	122.3 (3)	C5—C6—H6A	109.5
N1—C2—S1	115.4 (2)	C5—C6—H6B	109.5
N2—C2—S1	122.3 (2)	H6A—C6—H6B	109.5
C1—C3—C5	134.3 (3)	C5—C6—H6C	109.5
C1—C3—S1	109.7 (2)	H6A—C6—H6C	109.5
C5—C3—S1	116.0 (2)	H6B—C6—H6C	109.5
C1—C4—H4A	109.5	C2—N1—C1	110.7 (3)
C1—C4—H4B	109.5	C2—N2—H1A	120.0
H4A—C4—H4B	109.5	C2—N2—H1B	120.0
C1—C4—H4C	109.5	H1A—N2—H1B	120.0
H4A—C4—H4C	109.5	C2—S1—C3	88.60 (15)
H4B—C4—H4C	109.5		
N1—C1—C3—C5	−179.3 (4)	N2—C2—N1—C1	179.3 (3)
C4—C1—C3—C5	2.0 (7)	S1—C2—N1—C1	−0.5 (4)
N1—C1—C3—S1	0.0 (4)	C3—C1—N1—C2	0.3 (5)
C4—C1—C3—S1	−178.7 (3)	C4—C1—N1—C2	179.2 (3)
C1—C3—C5—O1	−179.5 (4)	N1—C2—S1—C3	0.4 (3)
S1—C3—C5—O1	1.3 (5)	N2—C2—S1—C3	−179.4 (3)
C1—C3—C5—C6	−0.1 (7)	C1—C3—S1—C2	−0.2 (3)
S1—C3—C5—C6	−179.4 (3)	C5—C3—S1—C2	179.2 (3)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the (N1/S1/C1–C3) 1,3-thiazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*A*···N1[i]	0.86	2.11	2.963 (4)	175
N2—H1*B*···O1[ii]	0.86	2.02	2.835 (4)	158
C4—H4*B*···*Cg*1[iii]	0.96	2.89	3.603 (4)	132

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*−1/2.