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1-[2-(Dimethylazaniumyl)ethyl]-1*H*-1,2,3,4-tetrazole-5-thiolateSadasivam Sharmila Tagore,^a Sivaraman Krishna,^a
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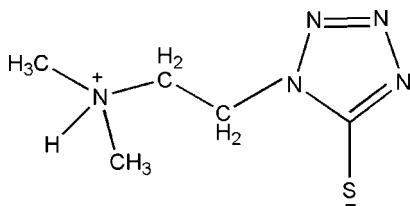
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.038; wR factor = 0.092; data-to-parameter ratio = 28.3.

In the crystal structure of the title zwitterion, $\text{C}_5\text{H}_{11}\text{N}_5\text{S}$, molecules are linked *via* $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds, forming zigzag chains propagating along [010]. The chains are linked by $\text{C}-\text{H}\cdots\text{S}$ hydrogen bonds, forming two dimensional networks lying parallel to (001).

Related literature

For the biological activity of tetrazoles, see: Juby *et al.* (1982); Tamilselvi & Mugesh (2009, 2011). For the general existence of zwitterions in other molecules and the involvement of a protonated N atom in hydrogen bonding, see: Ruanwas *et al.* (2012); Ha (2012). For the biological activity of cefotiam (systematic name: (6*R*,7*R*)-7-[[2-(2-amino-1,3-thiazol-4-yl)-acetyl]amino]-3-[[1-(2-dimethylaminoethyl)tetrazol-5-yl], an antibiotic with DMETT [1-(2-(dimethylamino)-ethyl)-1*H*-tetrazole-5-thione] as a side chain, against enterobacteriaceae, see: Garcia-Rodriguez *et al.* (1995); Polis & Tuazon (1985).



Experimental

Crystal data

$\text{C}_5\text{H}_{11}\text{N}_5\text{S}$
 $M_r = 173.26$
Monoclinic, $P2_1/c$
 $a = 7.1021$ (1) Å
 $b = 11.2476$ (2) Å
 $c = 10.7045$ (2) Å
 $\beta = 102.479$ (1)°

$V = 834.89$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.33$ mm⁻¹
 $T = 100$ K
0.41 × 0.21 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2004)
 $T_{\min} = 0.876$, $T_{\max} = 0.955$

11518 measured reflections
3004 independent reflections
2618 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.092$
 $S = 1.05$
3004 reflections
106 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N5}-\text{H5}\cdots\text{N4}^{\text{i}}$	0.934 (16)	1.889 (17)	2.8054 (14)	166.2 (16)
$\text{C4}-\text{H4C}\cdots\text{S1}^{\text{ii}}$	0.98	2.83	3.7275 (13)	153

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009), Mercury (Macrae *et al.*, 2008) and POV-RAY (Cason, 2004); software used to prepare material for publication: PLATON and publCIF (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: BV2228).

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supporting information

Acta Cryst. (2014). E70, o224 [doi:10.1107/S1600536814001573]

1-[2-(Dimethylazaniumyl)ethyl]-1*H*-1,2,3,4-tetrazole-5-thiolate

Sadasivam Sharmila Tagore, Sivaraman Krishna, Sundaramoorthy Gomathi and Velusamy Sethuraman

S1. Comment

A large number of tetrazole derivatives exhibit diverse pharmacological properties (Juby *et al.*, 1982) and some antibiotics with heterocyclic thiol side chains possess antithyroid activity (Tamilselvi & Mugesh, 2009). 1-(2-(Dimethylamino)-ethyl)-1*H*-tetrazole-5-thione (DMETT) exhibits thiol-thione tautomerism and thiolate anion formation which plays a vital role in the inhibition of the metallo- β -lactamases catalysed hydrolysis of cephalosporins (Tamilselvi & Mugesh, 2011). Cefotiam, a second-generation cephalosporin antibiotic, has a derivative of DMETT as a side chain which is more active against many of the Enterobacteriaceae including *Enterobacter*, *E-Coli*, *Klebsiella*, *Salmonella* and Indole-positive *Proteus* species (Garcia-Rodriguez *et al.* 1995; Polis & Tuazon, 1985).

The current investigation focusses on the supramolecular hydrogen bonded patterns exhibited by the title compound (Scheme. 1).

The title compound (I), 1-[2-(dimethylazaniumyl)ethyl]-1*H*-1,2,3,4-tetrazole-5-thiolate tetrazole-5-thiolate (DMATT) crystallizes with one molecule in the asymmetric unit and it exists as a zwitterion with the positive charge on the ammonium nitrogen atom and the negative charge on the thiolate sulfur atom (Fig 1).

This compound exists as a zwitterion like many other amino compounds reported in the literature (Ruanwas, *et al.*, 2012; Ha, 2012). There is an intramolecular exchange of thiol proton to amino nitrogen and thus thiolate formation, which leads to the generation of a nucleophilic sulfur species (responsible for the inhibition activity). The geometry of the *tert*- ammonium group is found to be tetrahedral with bond angles ranging from 106.9 (11)–113.32 (9)°. The maximum deviation of the side chain at N1 position from the mean plane of tetrazole ring moiety is found to be 0.313 (10) Å. The molecular confirmation is inferred from the torsion angles N1—C2—C3—N5, C2—C3—N5—C4 and C2—C3—N5—C5 and the values are found to be -81.52 (12)°, -166.23 (9)°, and 70.26 (12)° respectively.

Two inversion related zwitterions present in the same plane are linked by a strong N—H \cdots N hydrogen bond involving *tert*-ammonium group and ring N4ⁱ atom [symmetry code: $-x + 2, y - 1/2, -z + 1/2$] (Table 1). This interaction extends along *b* axis leading to the generation of a wave like supramolecular chain. The supramolecular chains in the adjacent planes are connected *via* a weak C—H \cdots S hydrogen bond. This hydrogen bond links one of the methyl C—H groups and S1ⁱⁱ atom [symmetry code: $x - 1, y, z$] and generates another wave like supramolecular chain extending along *a* axis. The centrosymmetric N—H \cdots N linkage between two zwitterions facilitates the effective occurrence of C—H \cdots S hydrogen bond thus forming a ring motif with a graph set of $R_4^4(23)$. This motif exists in both *a* and *b* axis and generates a two dimensional network as shown in Fig. 2.

S2. Experimental

The title compound was obtained by dissolving DMETT (Sigma-Aldrich; 43.3mg, 0.25 mmol) in 20 ml of hot methanol, warming the resultant solution over a water bath for half an hour and then keeping it at room temperature for crystallization. After a week's time, colorless prismatic crystals were obtained

S3. Refinement

The hydrogen atoms for the ammonium group (NH_4^+) was located in a difference Fourier map and refined freely. All other hydrogen atoms were positioned geometrically ($\text{C—H} = 0.98\text{--}0.99 \text{ \AA}$) and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH_2 or $1.5U_{\text{eq}}(\text{C})$ for CH_3 .

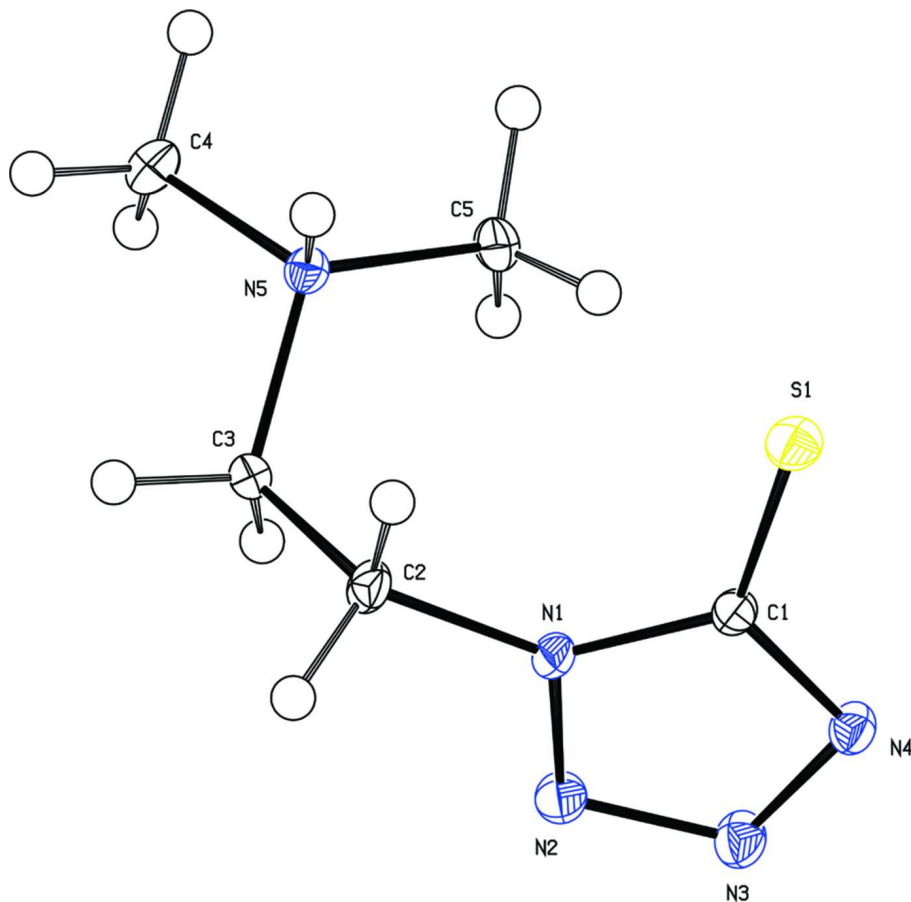


Figure 1

The asymmetric unit of (I), shown in 50% probability displacement ellipsoids.

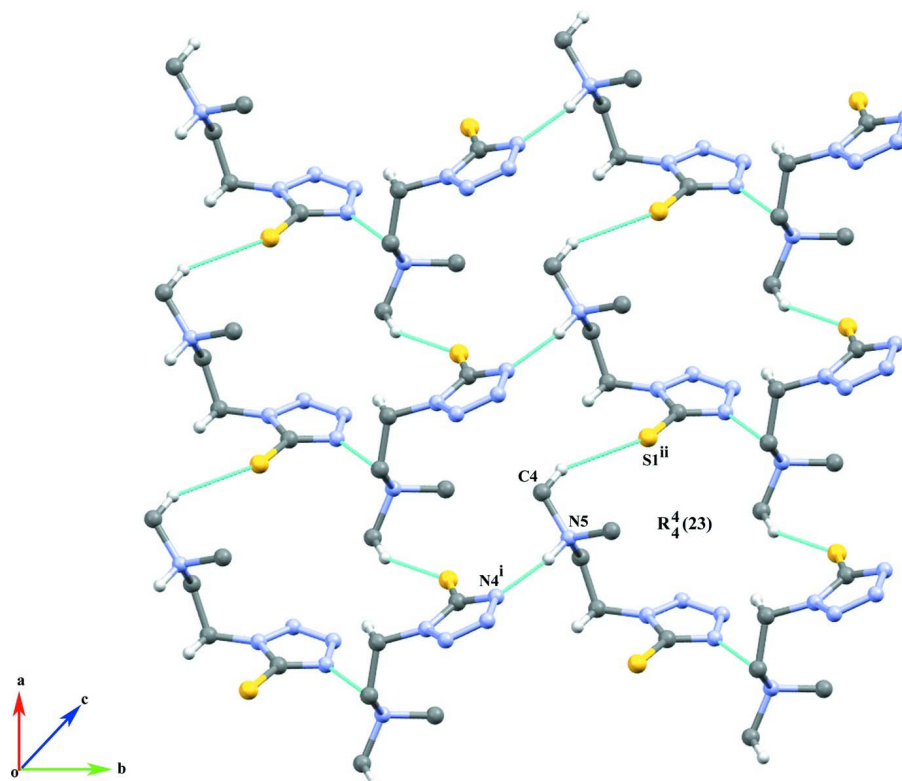


Figure 2

A view of two dimension network formed by N—H...N and C—H...S hydrogen bonds. [symmetry code: (i) $2 - x, -1/2 + y, 1/2 - z$; (ii) $-1 + x, y, z$].

1-[2-(Dimethylazanumyl)ethyl]-1*H*-1,2,3,4-tetrazole-5-thiolate

Crystal data

$C_5H_{11}N_5S$

$M_r = 173.26$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 7.1021$ (1) Å

$b = 11.2476$ (2) Å

$c = 10.7045$ (2) Å

$\beta = 102.479$ (1)°

$V = 834.89$ (2) Å³

$Z = 4$

$F(000) = 368$

$D_x = 1.378$ Mg m⁻³

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

Cell parameters from 3004 reflections

$\theta = 2.7$ – 32.7 °

$\mu = 0.33$ mm⁻¹

$T = 100$ K

Prism, colourless

$0.41 \times 0.21 \times 0.14$ mm

Data collection

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and φ scan

Absorption correction: multi-scan

(*SADABS*; Bruker, 2004)

$T_{\min} = 0.876$, $T_{\max} = 0.955$

11518 measured reflections

3004 independent reflections

2618 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 32.7$ °, $\theta_{\min} = 2.7$ °

$h = -10 \rightarrow 10$

$k = -16 \rightarrow 16$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.092$

$S = 1.05$

3004 reflections

106 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 atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.4372P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

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	1.21899 (4)	1.07521 (3)	0.25401 (3)	0.0158 (1)
N1	0.85227 (13)	1.05977 (8)	0.10942 (9)	0.0111 (2)
N2	0.71652 (14)	1.12926 (9)	0.03430 (9)	0.0146 (3)
N3	0.79116 (14)	1.23401 (9)	0.03491 (10)	0.0155 (3)
N4	0.97380 (13)	1.23578 (9)	0.10896 (9)	0.0129 (2)
N5	0.72606 (14)	0.90248 (8)	0.33382 (9)	0.0109 (2)
C1	1.01325 (15)	1.12532 (10)	0.15599 (10)	0.0112 (3)
C2	0.81956 (17)	0.93255 (10)	0.12032 (11)	0.0133 (3)
C3	0.66221 (16)	0.90062 (10)	0.19086 (10)	0.0120 (3)
C4	0.57703 (17)	0.84181 (11)	0.39090 (11)	0.0151 (3)
C5	0.76474 (17)	1.02474 (10)	0.38754 (10)	0.0137 (3)
H2A	0.94160	0.89510	0.16520	0.0160*
H2B	0.78540	0.89820	0.03320	0.0160*
H3A	0.55390	0.95710	0.16510	0.0140*
H3B	0.61320	0.82020	0.16390	0.0140*
H4A	0.61680	0.84390	0.48440	0.0230*
H4B	0.56360	0.75900	0.36190	0.0230*
H4C	0.45320	0.88280	0.36380	0.0230*
H5	0.839 (2)	0.8576 (16)	0.3566 (16)	0.024 (4)*
H5A	0.65260	1.07550	0.35540	0.0210*
H5B	0.87790	1.05780	0.36130	0.0210*
H5C	0.78910	1.02120	0.48110	0.0210*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0125 (1)	0.0164 (2)	0.0171 (1)	0.0012 (1)	0.0001 (1)	0.0039 (1)
N1	0.0124 (4)	0.0083 (4)	0.0120 (4)	-0.0003 (3)	0.0014 (3)	0.0014 (3)
N2	0.0142 (4)	0.0123 (5)	0.0155 (4)	0.0007 (4)	-0.0004 (3)	0.0024 (3)
N3	0.0141 (4)	0.0127 (5)	0.0186 (5)	0.0001 (4)	0.0009 (3)	0.0021 (3)
N4	0.0121 (4)	0.0106 (4)	0.0154 (4)	-0.0002 (3)	0.0020 (3)	0.0014 (3)
N5	0.0122 (4)	0.0089 (4)	0.0115 (4)	0.0003 (3)	0.0025 (3)	0.0003 (3)
C1	0.0132 (4)	0.0099 (5)	0.0110 (4)	-0.0007 (4)	0.0039 (3)	0.0000 (3)
C2	0.0185 (5)	0.0080 (5)	0.0144 (5)	-0.0018 (4)	0.0056 (4)	-0.0008 (4)
C3	0.0143 (5)	0.0108 (5)	0.0101 (4)	-0.0027 (4)	0.0012 (3)	-0.0006 (3)
C4	0.0162 (5)	0.0139 (5)	0.0166 (5)	-0.0007 (4)	0.0065 (4)	0.0028 (4)
C5	0.0170 (5)	0.0101 (5)	0.0137 (5)	-0.0014 (4)	0.0024 (4)	-0.0026 (4)

Geometric parameters (\AA , $^\circ$)

S1—C1	1.7003 (11)	C2—C3	1.5207 (17)
N1—N2	1.3609 (14)	C2—H2A	0.9900
N1—C1	1.3612 (14)	C2—H2B	0.9900
N1—C2	1.4584 (14)	C3—H3A	0.9900
N2—N3	1.2914 (14)	C3—H3B	0.9900
N3—N4	1.3664 (14)	C4—H4A	0.9800
N4—C1	1.3471 (15)	C4—H4B	0.9800
N5—C3	1.4994 (14)	C4—H4C	0.9800
N5—C4	1.4962 (16)	C5—H5A	0.9800
N5—C5	1.4929 (14)	C5—H5B	0.9800
N5—H5	0.934 (16)	C5—H5C	0.9800
S1...H2A	2.8400	C5...N1	3.1945 (14)
S1...H3A ⁱ	3.0500	C5...N3 ^x	3.1239 (15)
S1...H4C ⁱ	2.8300	C1...H5B	2.6900
S1...H5A ⁱ	3.0400	C1...H5 ⁱⁱ	2.830 (18)
S1...H5B	2.9000	C1...H2B ⁱⁱⁱ	2.7300
S1...H3B ⁱⁱ	3.0600	C2...H5B	2.8900
S1...H4B ⁱⁱ	3.0000	H2A...S1	2.8400
S1...H2B ⁱⁱⁱ	3.0800	H2A...H5	2.3600
S1...H4A ^{iv}	2.9400	H2B...S1 ⁱⁱⁱ	3.0800
S1...H5C ^{iv}	3.0500	H2B...N4 ⁱⁱⁱ	2.9400
N1...N4	2.1601 (14)	H2B...C1 ⁱⁱⁱ	2.7300
N1...N5	3.2610 (13)	H3A...S1 ^{xi}	3.0500
N1...C5	3.1945 (14)	H3A...N2	2.7800
N2...C4 ^v	3.3800 (16)	H3A...H4C	2.5300
N2...N4	2.1867 (14)	H3A...H5A	2.4100
N2...C3 ^{vi}	3.2180 (15)	H3A...N2 ^{vi}	2.7200
N3...C5 ^{vii}	3.1239 (15)	H3B...H4B	2.3300
N3...C4 ^v	3.1363 (16)	H3B...S1 ^{viii}	3.0600
N4...C4 ⁱⁱ	3.4054 (16)	H3B...N2 ^{vi}	2.8600

N4...N1	2.1601 (14)	H4A...H5C	2.3400
N4...N5 ⁱⁱ	2.8054 (14)	H4A...S1 ^{iv}	2.9400
N5...N1	3.2610 (13)	H4B...H3B	2.3300
N5...N4 ^{viii}	2.8054 (14)	H4B...S1 ^{viii}	3.0000
N1...H5B	2.6600	H4B...N2 ^{ix}	2.8800
N2...H3A	2.7800	H4C...S1 ^{xi}	2.8300
N2...H4B ^v	2.8800	H4C...H3A	2.5300
N2...H3A ^{vi}	2.7200	H4C...N3 ^{ix}	2.7900
N2...H3B ^{vi}	2.8600	H5...H2A	2.3600
N3...H4C ^v	2.7900	H5...N4 ^{viii}	1.889 (17)
N3...H5C ^{vii}	2.8100	H5...C1 ^{viii}	2.830 (18)
N3...H5A ^{vii}	2.9000	H5A...S1 ^{xi}	3.0400
N4...H2B ⁱⁱⁱ	2.9400	H5A...H3A	2.4100
N4...H5 ⁱⁱ	1.889 (17)	H5A...N3 ^x	2.9000
C1...C5	3.5255 (16)	H5B...S1	2.9000
C1...C2 ⁱⁱⁱ	3.4785 (16)	H5B...N1	2.6600
C2...C1 ⁱⁱⁱ	3.4785 (16)	H5B...C1	2.6900
C3...N2 ^{vi}	3.2180 (15)	H5B...C2	2.8900
C4...N3 ^{ix}	3.1363 (16)	H5C...H4A	2.3400
C4...N2 ^{ix}	3.3800 (16)	H5C...S1 ^{iv}	3.0500
C4...N4 ^{viii}	3.4054 (16)	H5C...N3 ^x	2.8100
C5...C1	3.5255 (16)		
N2—N1—C1	109.70 (9)	C3—C2—H2B	109.00
N2—N1—C2	120.40 (9)	H2A—C2—H2B	108.00
C1—N1—C2	129.63 (10)	N5—C3—H3A	109.00
N1—N2—N3	106.46 (9)	N5—C3—H3B	109.00
N2—N3—N4	110.70 (9)	C2—C3—H3A	109.00
N3—N4—C1	107.34 (9)	C2—C3—H3B	109.00
C3—N5—C4	109.02 (9)	H3A—C3—H3B	108.00
C3—N5—C5	113.32 (8)	N5—C4—H4A	109.00
C4—N5—C5	110.51 (9)	N5—C4—H4B	109.00
C5—N5—H5	108.7 (11)	N5—C4—H4C	109.00
C3—N5—H5	108.2 (10)	H4A—C4—H4B	109.00
C4—N5—H5	106.9 (10)	H4A—C4—H4C	109.00
S1—C1—N4	128.17 (9)	H4B—C4—H4C	109.00
S1—C1—N1	126.03 (9)	N5—C5—H5A	109.00
N1—C1—N4	105.80 (9)	N5—C5—H5B	109.00
N1—C2—C3	114.73 (9)	N5—C5—H5C	109.00
N5—C3—C2	114.26 (9)	H5A—C5—H5B	109.00
N1—C2—H2A	109.00	H5A—C5—H5C	109.00
N1—C2—H2B	109.00	H5B—C5—H5C	109.00
C3—C2—H2A	109.00		
C1—N1—N2—N3	-0.17 (12)	N1—N2—N3—N4	-0.04 (12)
C2—N1—N2—N3	-174.75 (10)	N2—N3—N4—C1	0.24 (12)
N2—N1—C1—S1	179.98 (9)	N3—N4—C1—S1	-180.00 (8)
N2—N1—C1—N4	0.31 (12)	N3—N4—C1—N1	-0.33 (12)

C2—N1—C1—S1	-6.09 (17)	C4—N5—C3—C2	-166.23 (9)
C2—N1—C1—N4	174.24 (10)	C5—N5—C3—C2	70.26 (12)
N2—N1—C2—C3	-68.63 (13)	N1—C2—C3—N5	-81.52 (12)
C1—N1—C2—C3	118.00 (12)		

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+2, y+1/2, -z+1/2$; (iii) $-x+2, -y+2, -z$; (iv) $-x+2, -y+2, -z+1$; (v) $-x+1, y+1/2, -z+1/2$; (vi) $-x+1, -y+2, -z$; (vii) $x, -y+5/2, z-1/2$; (viii) $-x+2, y-1/2, -z+1/2$; (ix) $-x+1, y-1/2, -z+1/2$; (x) $x, -y+5/2, z+1/2$; (xi) $x-1, y, z$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N5—H5 \cdots N4 ^{viii}	0.934 (16)	1.889 (17)	2.8054 (14)	166.2 (16)
C2—H2A \cdots S1	0.99	2.84	3.3039 (12)	109
C4—H4C \cdots S1 ^{xi}	0.98	2.83	3.7275 (13)	153

Symmetry codes: (viii) $-x+2, y-1/2, -z+1/2$; (xi) $x-1, y, z$.