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# *N*-Methylpyrrolidine-1-carbothioamide

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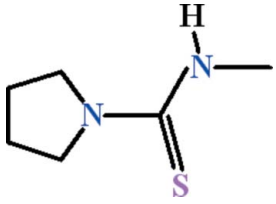
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.011 Å; $R$ factor = 0.079; $wR$ factor = 0.262; data-to-parameter ratio = 16.4.

There are two independent molecules in the asymmetric unit of the title compound, $C_6H_{12}N_2S$, in which the *N*-methylthioformamide unit and the pyrrolidine ring mean plane are oriented at dihedral angles of 5.9 (5) and 5.9 (4)°. In the crystal, zigzag $C(4)$ chains extending along the *a* axis are formed due to N—H···S hydrogen bonds between alternate arrangements of molecules. The chains are interlinked by C—H···S hydrogen bonds.

## Related literature

For a related structure, see: Jiang (2009). For graph–set notation, see: Bernstein *et al.* (1995).




## Experimental

### *Crystal data*

$C_6H_{12}N_2S$
$M_r$ = 144.25
Triclinic, $P\overline{1}$
$a$ = 8.616 (2) Å
$b$ = 9.077 (2) Å
$c$ = 10.796 (3) Å
$\alpha$ = 73.725 (14)°
$\beta$ = 86.656 (15)°
$\gamma$ = 76.177 (16)°
$V$ = 787.0 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.33 mm$^{-1}$
$T$ = 296 K
0.30 × 0.25 × 0.20 mm

### *Data collection*

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.957, $T_{max}$ = 0.966
9119 measured reflections
2699 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.262
$S$ = 1.04
2699 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···S2$^{i}$ | 0.86 | 2.73 | 3.472 (5) | 145 |
| N3—H4···S1$^{ii}$ | 0.86 | 2.64 | 3.410 (5) | 150 |
| C12—H12*B*···S1$^{iii}$ | 0.97 | 2.84 | 3.765 (5) | 159 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $x, y, z+1$.

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*.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan. MNU, MS, AA and IK also gratefully acknowledge the financial support provided by the Higher Education Commission (HEC), Islamabad, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2355).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1706 [doi:10.1107/S1600536812020971]

## *N*-Methylpyrrolidine-1-carbothioamide

**M. Naveed Umar, M. Nawaz Tahir, Mohammad Shoaib, Akbar Ali and Imran Khan**

### Comment

The title compound (I), (Fig. 1) has been synthesized as a derivative. The crystal structure of *N*-phenylpyrrolidine-1-carbothioamide related to this structure (I) has been published previously (Jiang, 2009). In (I), two molecules in the asymmetric unit are present, which differ slightly from each other geometrically. In one molecule, the *N*-methylthioformamide moiety A (C1/N1/C2/S1) and the pyrrolidine ring B (N2/C3–C6) are planar with r.m.s. deviation of 0.0010 Å and 0.0360 Å, respectively. The dihedral angle between A/B is 5.88 (46)°. In second molecule, the similar groups C (C7/N3/C8/S2) and D (N4/C9—C12) are also planar with r.m.s. deviation of 0.0032 Å and 0.0839 Å, respectively and the dihedral angle between C/D is 5.92 (39)°. Both molecules are interlinked through classical intramolecular H–bonding of N—H···S type (Table 1, Fig. 2) with *C*(4) chains (Bernstein *et al.*, 1995) to form zigzag infinite one-dimensional polymeric chains extending along the *a*-axis. The polymeric chains are interlinked due to C—H···S type of H–bonding (Table 1, Fig. 2).

### Experimental

A solution of pyrrolidine (0.36 g, 5.00 mmol) in $CH_3CN$ (3 ml) was added dropwise to a stirred solution of methyl isothiocyanate (0.47 ml, 5.50 mmol) in $CH_3CN$ (10 ml, anhydrous) under cooling in an ice-bath to keep the reaction temperature below 283 K. The ice-bath was removed and stirring was continued at room temperature for 2 h to furnish a yellow-colored solution. The reaction mixture was extracted with ethylacetate and subjected to column chromatography to get the colorless product in 67% yield and then recrystalized with methanol to get colorless prisms of (I).

### Refinement

The H-atoms were positioned geometrically (C–H = 0.96–0.97 Å, N—H = 0.86 Å) and refined as riding with $U_{iso}$(H) = $xU_{eq}$(C, N), where $x$ = 1.5 for methyl and $x$ = 1.2 for all 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).

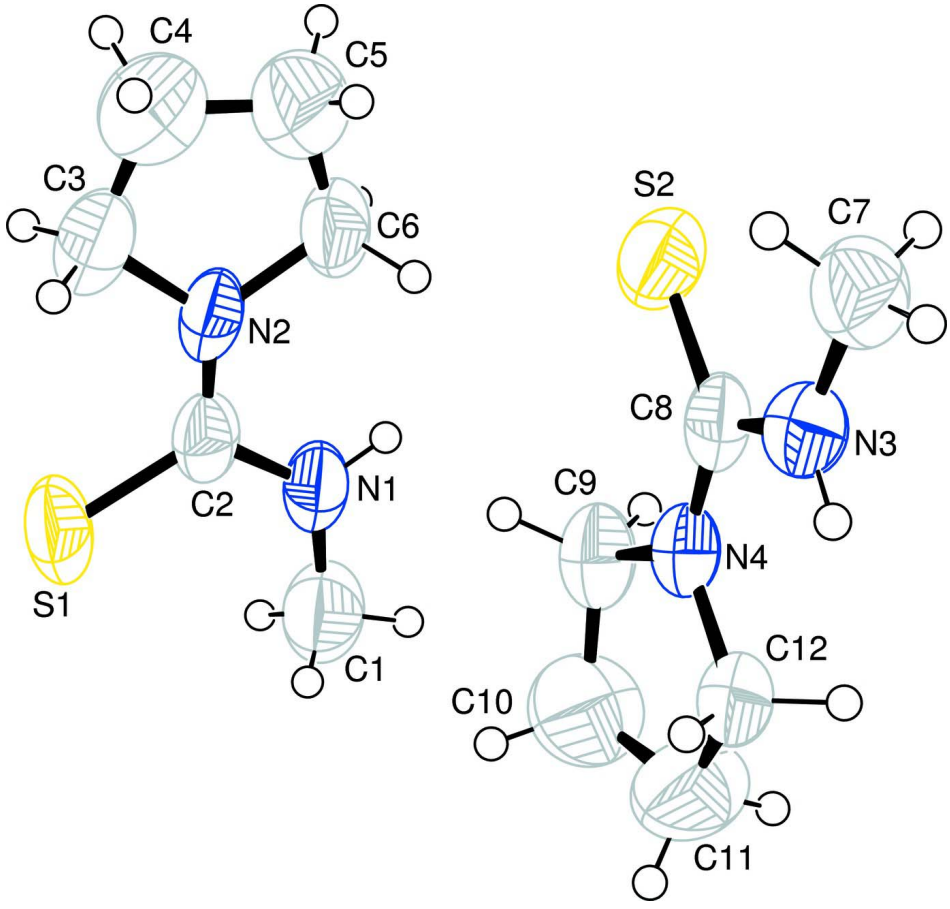


**Figure 1**

View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

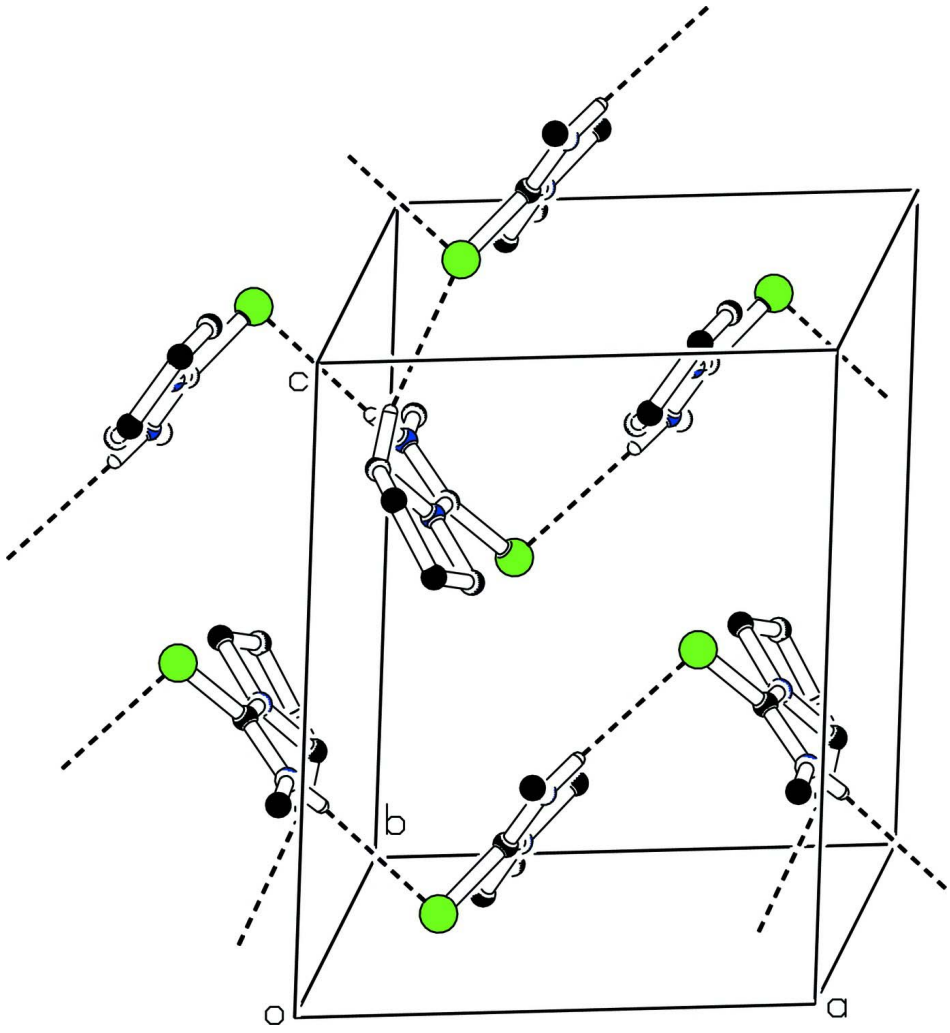


**Figure 2**

The partial packing (*PLATON*; Spek, 2009) which shows that molecules are interlinked to form polymeric chains along the *a*-axis. The H-atoms not involved in H-bonding are omitted for clarity.

### *N*-Methylpyrrolidine-1-carbothioamide

*Crystal data*

$C_6H_{12}N_2S$
$M_r = 144.25$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.616$ (2) Å
$b = 9.077$ (2) Å
$c = 10.796$ (3) Å
$\alpha = 73.725$ (14)°
$\beta = 86.656$ (15)°
$\gamma = 76.177$ (16)°
$V = 787.0$ (3) Å$^3$
$Z = 4$
$F(000) = 312$
$D_x = 1.217$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1204 reflections
$\theta = 2.4$–26.0°
$\mu = 0.33$ mm$^{-1}$
$T = 296$ K
Prism, colorless
0.30 × 0.25 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.957, $T_{max}$ = 0.966
9119 measured reflections
2699 independent reflections
1385 reflections with $I > 3\sigma(I)$
$R_{int}$ = 0.067
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.4°
$h$ = −10→10
$k$ = −11→11
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.262
$S$ = 1.04
2699 reflections
165 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
$w = 1/[\sigma^2(F_o^2) + (0.1268P)^2 + 0.3916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4239 (8) | 0.1340 (7) | 0.3083 (6) | 0.101 (2) |
| H1A | 0.3186 | 0.1209 | 0.3350 | 0.151* |
| H1B | 0.4965 | 0.0862 | 0.3803 | 0.151* |
| H1C | 0.4586 | 0.0844 | 0.2406 | 0.151* |
| C2 | 0.3360 (6) | 0.3972 (7) | 0.1594 (5) | 0.0699 (14) |
| C3 | 0.2574 (7) | 0.6685 (8) | 0.0191 (5) | 0.0913 (18) |
| H3A | 0.2961 | 0.6484 | −0.0622 | 0.110* |
| H3B | 0.1437 | 0.6732 | 0.0248 | 0.110* |
| C4 | 0.2906 (12) | 0.8143 (10) | 0.0304 (9) | 0.153 (3) |
| H4A | 0.3452 | 0.8611 | −0.0463 | 0.184* |
| H4B | 0.1906 | 0.8885 | 0.0365 | 0.184* |
| C5 | 0.3868 (11) | 0.7860 (8) | 0.1411 (7) | 0.123 (3) |
| H5A | 0.3265 | 0.8361 | 0.2030 | 0.148* |
| H5B | 0.4801 | 0.8297 | 0.1166 | 0.148* |
| C6 | 0.4365 (7) | 0.6143 (7) | 0.1987 (5) | 0.0846 (17) |
| H6A | 0.4123 | 0.5869 | 0.2900 | 0.101* |

| | | | | |
|---|---|---|---|---|
| H6B | 0.5503 | 0.5764 | 0.1880 | 0.101* |
| C7 | 0.0612 (8) | 0.8849 (7) | 0.7020 (6) | 0.0905 (18) |
| H7A | 0.1661 | 0.8968 | 0.7156 | 0.136* |
| H7B | −0.0082 | 0.9109 | 0.7695 | 0.136* |
| H7C | 0.0199 | 0.9542 | 0.6202 | 0.136* |
| C8 | 0.1664 (6) | 0.6492 (6) | 0.6253 (4) | 0.0668 (14) |
| C9 | 0.2534 (7) | 0.4014 (7) | 0.5615 (5) | 0.0791 (15) |
| H9A | 0.3672 | 0.3846 | 0.5754 | 0.095* |
| H9B | 0.2292 | 0.4497 | 0.4704 | 0.095* |
| C10 | 0.2012 (10) | 0.2515 (9) | 0.6076 (8) | 0.126 (3) |
| H10A | 0.1297 | 0.2437 | 0.5447 | 0.151* |
| H10B | 0.2930 | 0.1627 | 0.6193 | 0.151* |
| C11 | 0.1210 (11) | 0.2487 (8) | 0.7269 (7) | 0.125 (3) |
| H11A | 0.1933 | 0.1864 | 0.7980 | 0.150* |
| H11B | 0.0307 | 0.2009 | 0.7314 | 0.150* |
| C12 | 0.0651 (7) | 0.4120 (6) | 0.7365 (5) | 0.0768 (15) |
| H12A | −0.0481 | 0.4515 | 0.7165 | 0.092* |
| H12B | 0.0846 | 0.4183 | 0.8222 | 0.092* |
| N1 | 0.4210 (5) | 0.2971 (5) | 0.2626 (4) | 0.0771 (13) |
| H1 | 0.4775 | 0.3348 | 0.3037 | 0.093* |
| N2 | 0.3437 (5) | 0.5463 (6) | 0.1280 (4) | 0.0739 (12) |
| N3 | 0.0697 (5) | 0.7250 (5) | 0.7032 (4) | 0.0746 (12) |
| H4 | 0.0100 | 0.6740 | 0.7564 | 0.089* |
| N4 | 0.1603 (5) | 0.5002 (5) | 0.6404 (4) | 0.0677 (11) |
| S1 | 0.22218 (19) | 0.3304 (2) | 0.07310 (14) | 0.0932 (6) |
| S2 | 0.28575 (19) | 0.74016 (18) | 0.51593 (13) | 0.0881 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.122 (5) | 0.099 (5) | 0.083 (4) | −0.026 (4) | −0.013 (4) | −0.024 (4) |
| C2 | 0.071 (3) | 0.102 (4) | 0.040 (3) | −0.018 (3) | 0.003 (2) | −0.027 (3) |
| C3 | 0.087 (4) | 0.116 (5) | 0.060 (3) | −0.020 (4) | −0.009 (3) | −0.007 (3) |
| C4 | 0.202 (10) | 0.116 (6) | 0.127 (7) | −0.046 (6) | −0.058 (7) | 0.007 (5) |
| C5 | 0.180 (8) | 0.100 (5) | 0.095 (5) | −0.040 (5) | −0.017 (5) | −0.025 (4) |
| C6 | 0.102 (4) | 0.107 (5) | 0.052 (3) | −0.030 (4) | −0.004 (3) | −0.027 (3) |
| C7 | 0.115 (5) | 0.085 (4) | 0.078 (4) | −0.024 (3) | 0.000 (3) | −0.032 (3) |
| C8 | 0.071 (3) | 0.088 (4) | 0.042 (3) | −0.018 (3) | −0.014 (2) | −0.016 (3) |
| C9 | 0.081 (4) | 0.100 (4) | 0.061 (3) | −0.013 (3) | −0.001 (3) | −0.035 (3) |
| C10 | 0.154 (7) | 0.104 (5) | 0.136 (7) | −0.036 (5) | 0.023 (6) | −0.061 (5) |
| C11 | 0.187 (8) | 0.088 (5) | 0.109 (6) | −0.044 (5) | 0.038 (5) | −0.036 (4) |
| C12 | 0.093 (4) | 0.096 (4) | 0.050 (3) | −0.038 (3) | 0.000 (3) | −0.021 (3) |
| N1 | 0.088 (3) | 0.093 (3) | 0.054 (3) | −0.023 (3) | −0.011 (2) | −0.022 (2) |
| N2 | 0.081 (3) | 0.098 (3) | 0.041 (2) | −0.020 (3) | −0.009 (2) | −0.017 (2) |
| N3 | 0.090 (3) | 0.086 (3) | 0.055 (3) | −0.031 (2) | 0.008 (2) | −0.023 (2) |
| N4 | 0.083 (3) | 0.080 (3) | 0.045 (2) | −0.021 (2) | −0.001 (2) | −0.023 (2) |
| S1 | 0.0962 (12) | 0.1408 (15) | 0.0594 (9) | −0.0374 (10) | −0.0056 (8) | −0.0447 (9) |
| S2 | 0.0935 (12) | 0.1108 (13) | 0.0601 (9) | −0.0357 (9) | 0.0018 (8) | −0.0135 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.418 (7) | C7—H7A | 0.9600 |
| C1—H1A | 0.9600 | C7—H7B | 0.9600 |
| C1—H1B | 0.9600 | C7—H7C | 0.9600 |
| C1—H1C | 0.9600 | C8—N4 | 1.330 (6) |
| C2—N2 | 1.316 (6) | C8—N3 | 1.358 (6) |
| C2—N1 | 1.346 (6) | C8—S2 | 1.688 (5) |
| C2—S1 | 1.705 (5) | C9—N4 | 1.475 (6) |
| C3—C4 | 1.457 (9) | C9—C10 | 1.480 (9) |
| C3—N2 | 1.464 (7) | C9—H9A | 0.9700 |
| C3—H3A | 0.9700 | C9—H9B | 0.9700 |
| C3—H3B | 0.9700 | C10—C11 | 1.422 (10) |
| C4—C5 | 1.423 (10) | C10—H10A | 0.9700 |
| C4—H4A | 0.9700 | C10—H10B | 0.9700 |
| C4—H4B | 0.9700 | C11—C12 | 1.476 (8) |
| C5—C6 | 1.473 (8) | C11—H11A | 0.9700 |
| C5—H5A | 0.9700 | C11—H11B | 0.9700 |
| C5—H5B | 0.9700 | C12—N4 | 1.462 (6) |
| C6—N2 | 1.474 (6) | C12—H12A | 0.9700 |
| C6—H6A | 0.9700 | C12—H12B | 0.9700 |
| C6—H6B | 0.9700 | N1—H1 | 0.8600 |
| C7—N3 | 1.432 (6) | N3—H4 | 0.8600 |
| | | | |
| N1—C1—H1A | 109.5 | N4—C8—N3 | 115.8 (5) |
| N1—C1—H1B | 109.5 | N4—C8—S2 | 122.6 (4) |
| H1A—C1—H1B | 109.5 | N3—C8—S2 | 121.6 (4) |
| N1—C1—H1C | 109.5 | N4—C9—C10 | 103.7 (5) |
| H1A—C1—H1C | 109.5 | N4—C9—H9A | 111.0 |
| H1B—C1—H1C | 109.5 | C10—C9—H9A | 111.0 |
| N2—C2—N1 | 118.2 (4) | N4—C9—H9B | 111.0 |
| N2—C2—S1 | 121.6 (4) | C10—C9—H9B | 111.0 |
| N1—C2—S1 | 120.2 (4) | H9A—C9—H9B | 109.0 |
| C4—C3—N2 | 104.4 (5) | C11—C10—C9 | 108.4 (6) |
| C4—C3—H3A | 110.9 | C11—C10—H10A | 110.0 |
| N2—C3—H3A | 110.9 | C9—C10—H10A | 110.0 |
| C4—C3—H3B | 110.9 | C11—C10—H10B | 110.0 |
| N2—C3—H3B | 110.9 | C9—C10—H10B | 110.0 |
| H3A—C3—H3B | 108.9 | H10A—C10—H10B | 108.4 |
| C5—C4—C3 | 111.2 (6) | C10—C11—C12 | 108.9 (6) |
| C5—C4—H4A | 109.4 | C10—C11—H11A | 109.9 |
| C3—C4—H4A | 109.4 | C12—C11—H11A | 109.9 |
| C5—C4—H4B | 109.4 | C10—C11—H11B | 109.9 |
| C3—C4—H4B | 109.4 | C12—C11—H11B | 109.9 |
| H4A—C4—H4B | 108.0 | H11A—C11—H11B | 108.3 |
| C4—C5—C6 | 108.3 (6) | N4—C12—C11 | 103.6 (5) |
| C4—C5—H5A | 110.0 | N4—C12—H12A | 111.0 |
| C6—C5—H5A | 110.0 | C11—C12—H12A | 111.0 |
| C4—C5—H5B | 110.0 | N4—C12—H12B | 111.0 |
| C6—C5—H5B | 110.0 | C11—C12—H12B | 111.0 |

| | | | |
|---|---|---|---|
| H5A—C5—H5B | 108.4 | H12A—C12—H12B | 109.0 |
| C5—C6—N2 | 104.9 (5) | C2—N1—C1 | 124.6 (5) |
| C5—C6—H6A | 110.8 | C2—N1—H1 | 117.7 |
| N2—C6—H6A | 110.8 | C1—N1—H1 | 117.7 |
| C5—C6—H6B | 110.8 | C2—N2—C3 | 124.3 (5) |
| N2—C6—H6B | 110.8 | C2—N2—C6 | 125.1 (4) |
| H6A—C6—H6B | 108.8 | C3—N2—C6 | 110.6 (5) |
| N3—C7—H7A | 109.5 | C8—N3—C7 | 123.9 (5) |
| N3—C7—H7B | 109.5 | C8—N3—H4 | 118.0 |
| H7A—C7—H7B | 109.5 | C7—N3—H4 | 118.0 |
| N3—C7—H7C | 109.5 | C8—N4—C12 | 125.5 (4) |
| H7A—C7—H7C | 109.5 | C8—N4—C9 | 123.2 (4) |
| H7B—C7—H7C | 109.5 | C12—N4—C9 | 111.3 (4) |
| | | | |
| N2—C3—C4—C5 | −1.7 (10) | C4—C3—N2—C6 | −4.0 (7) |
| C3—C4—C5—C6 | 6.6 (11) | C5—C6—N2—C2 | −170.9 (6) |
| C4—C5—C6—N2 | −8.6 (8) | C5—C6—N2—C3 | 7.8 (6) |
| N4—C9—C10—C11 | −15.4 (8) | N4—C8—N3—C7 | 179.3 (5) |
| C9—C10—C11—C12 | 21.4 (10) | S2—C8—N3—C7 | −1.0 (7) |
| C10—C11—C12—N4 | −17.9 (8) | N3—C8—N4—C12 | −3.0 (7) |
| N2—C2—N1—C1 | 179.6 (5) | S2—C8—N4—C12 | 177.3 (4) |
| S1—C2—N1—C1 | −0.3 (7) | N3—C8—N4—C9 | 178.1 (4) |
| N1—C2—N2—C3 | −179.7 (5) | S2—C8—N4—C9 | −1.6 (6) |
| S1—C2—N2—C3 | 0.3 (7) | C11—C12—N4—C8 | −170.9 (5) |
| N1—C2—N2—C6 | −1.1 (8) | C11—C12—N4—C9 | 8.1 (6) |
| S1—C2—N2—C6 | 178.8 (4) | C10—C9—N4—C8 | −176.9 (5) |
| C4—C3—N2—C2 | 174.7 (6) | C10—C9—N4—C12 | 4.1 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···S2$^{i}$ | 0.86 | 2.73 | 3.472 (5) | 145 |
| N3—H4···S1$^{ii}$ | 0.86 | 2.64 | 3.410 (5) | 150 |
| C12—H12*B*···S1$^{iii}$ | 0.97 | 2.84 | 3.765 (5) | 159 |

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