1-(Cycloheptylidene)thiosemicarbazide

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The asymmetric unit of the title compound, $C_8H_{15}N_3S$, contains two independent molecules. In both molecules, the seven-membered cycloheptane ring adopts a chair conformation. An intramolecular N—H···N hydrogen bond is observed in both molecules, forming $S(5)$ graph-set motifs. In the crystal, the two independent molecules are connected through N—H···S hydrogen bonds, forming dimers which are in turn further connected by N—H···S hydrogen bonds into chains along [010].

3D view

Chemical scheme
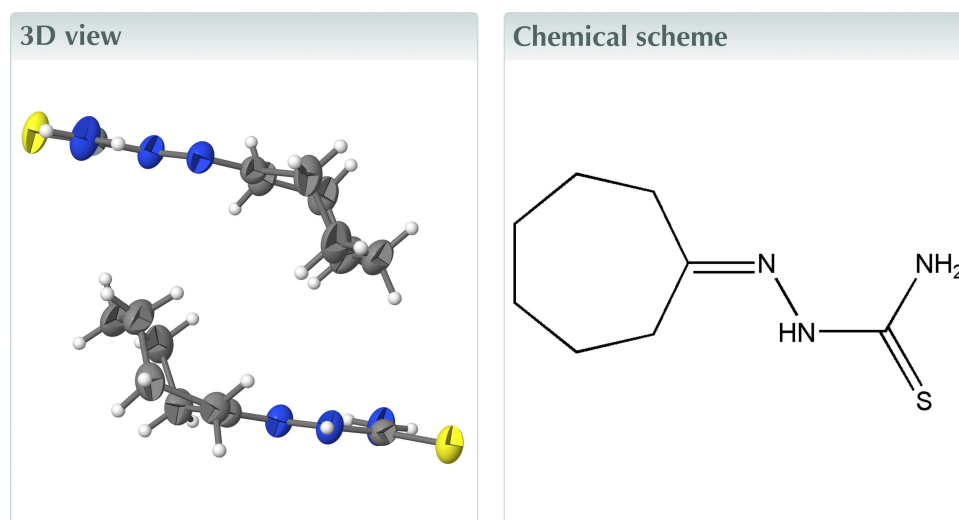
Structure description

Thiosemicarbazones constitute an important class of *N*,*S*-donor ligands and their coordination chemistry was initially explored in the early 1960 s (Gingras *et al.*, 1961; Ali & Livingstone, 1974; Lobana *et al.*, 2009). Thiocarbazones and their metal complexes have received considerable research interest owing to their medicinal properties, such as antifungal (Arjmand *et al.*, 2007), anticancer (Sharma *et al.*, 2006), antibacterial (Singh *et al.*, 2008), antiviral (Padmanabhan *et al.*, 2017) and antimalarial (Oliveira *et al.*, 2008). Based on these observations, we report herein the synthesis and crystal structure of the title compound.

The asymmetric unit of the crystal structure contains two independent molecules (Fig. 1). All bond lengths are within normal ranges (Allen *et al.*, 1987) and are comparable with a related structure (Akkurt *et al.*, 2014). The cycloheptane ring adopts a chair conformation in both molecules (Duax & Norton, 1975), with the best mirror plane passing through atom C6*A* and bisecting the C2*A*—C3*A* bond in molecule *A* [asymmetry parameter $\Delta Cs(6A) = 2.07$], whereas in molecule *B*, the mirror plane passes through atom C5*B* and bisects the C2*B*—C8*B* bond [asymmetry parameter $\Delta Cs(5B) = 11.11$]. Intramolecular N—H···N hydrogen bonds are observed in both molecules (Table 1), forming an $S(5)$ graph-set motif. In the crystal, pairs of molecules form dimers (Fig. 2) through N—H···S hydrogen bonds, forming an $R_2^2(8)$ graph-set motif (Bernstein *et al.*,

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1A—H1A1⋯N3A	0.86	2.22	2.5943 (2)	106
N1B—H1B1⋯N3B	0.86	2.22	2.5904 (2)	106
N1A—H1A2⋯S1B^i	0.86	2.64	3.4642 (2)	160
N1B—H1B2⋯S1A^{ii}	0.86	2.53	3.3499 (2)	161
N2B—H2B⋯S1A^{iii}	0.86	2.87	3.6254 (2)	147

Symmetry codes: (i) $x, y, z - 1$; (ii) $x, y, z + 1$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

1995). These dimers are further connected by N—H⋯S hydrogen bonds, forming chains along [010] (Fig. 2).

Synthesis and crystallization

A mixture of cycloheptanone (1 mmol) and thiosemicarbazide (1 mmol) in aqueous ethanol (50:50 v/v, 5 ml) was stirred at room temperature for 2 h until completion of the reaction monitored by thin-layer chromatography. The solid product obtained was isolated by simple filtration and X-ray-quality crystals were grown from a solution in ethanol. The desired 1-(cycloheptylidene)thiosemicarbazide was characterized by NMR and mass spectral data.

IR (KBr): 3380, 3286, 2987, 1586, 1454, 1085 cm^{-1}. [1] H NMR (CDCl$_3$, 300 MHz): δ 1.68 (d, 5H), 1.77 (s, 3H), 2.48–2.37 (m, 4H), 7.27 (s, 1H), 8.4 (s, 2H). MS(EI): (m/z) 185.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and were treated as riding on their parent C or N atoms, with C—H = 0.97 Å and N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.
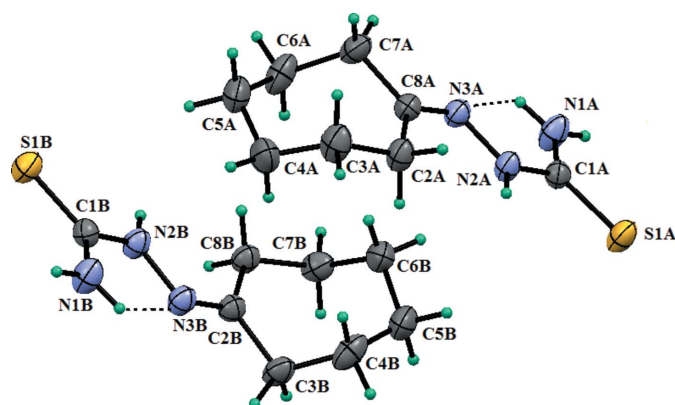
Funding information

Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

Table 2
Experimental details.

Crystal data	
Chemical formula	C$_8$H$_{15}$N$_3$S
M_r	185.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	12.7584 (8), 11.7060 (7), 13.3452 (8)
β (°)	92.273 (2)
V (Å^3)	1991.5 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker Xcalibur Sapphire3
Absorption correction	Multi-scan (SADABS; Bruker, 2004)
T_{min}, T_{max}	0.699, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33823, 3912, 3464
R_{int}	0.024
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.091, 1.06
No. of reflections	3912
No. of parameters	217
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.26

Computer programs: APEX2 (Bruker 2004), SAINT (Bruker 2004), SHELXS97 (Sheldrick, 2008), SHELXL2016 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009).

References

Akkurt, M., Mohamed, S. K., Mague, J. T., Hassan, A. A. & Albayati, M. R. (2014). Acta Cryst. E**70**, o359.

Ali, M. A. & Livingstone, S. E. (1974). Coord. Chem. Rev. **13**, 101–132.

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Prpen, A. G. & Taylor, R. (1987). J. Chem. Soc. Perkin Trans. 2, pp. S1–19.
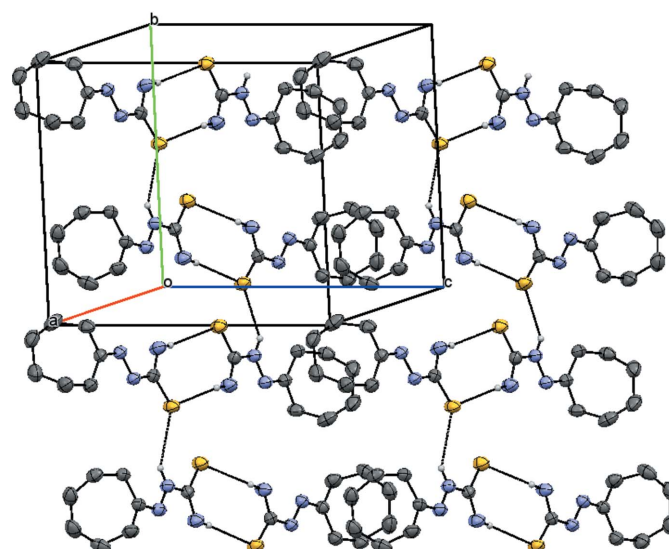
Figure 2
Part of the crystal structure, with hydrogen bonds shown as dotted lines.

Arjmand, F., Mohani, B. & Ahmad, S. (2007). *Eur. J. Med. Chem.* **40**, 1103–1110.

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

Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Duax, W. L. & Norton, D. A. (1975). *Atlas of Steroid Structures*, Vol. 1. New York: Plenum Press.

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

Gingras, B. A., Somorjai, R. L. & Bayley, C. H. (1961). *Can. J. Chem.* **39**, 973–985.

Lobana, T. S., Sharma, R., Bawa, G. & Khanna, S. (2009). *Coord. Chem. Rev.* **253**, 977–1055.

Oliveira, R. B. de, deSouza-Fagundes, E. M., Soares, R. P., Andrade, A. A., Krettli, A. U. & Zani, C. L. (2008). *Eur. J. Med. Chem.* **43**, 1983–1988.

Padmanabhan, P., Khaleefathullah, S., Kaveri, K., Palani, G., Ramanathan, G., Thennarasu, S. & Sivagnanam, U. T. (2017). *J. Med. Virol.* **89**, 546–552.

Sharma, R., Agarwal, S. K., Rawat, S. & Nagar, M. (2006). *Transition Met. Chem.* **31**, 201–206.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

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

Singh, K., Barwa, M. S. & Tyagi, P. (2008). *Eur. J. Med. Chem.* **42**, 394–402.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

full crystallographic data

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Crystal data

$C_8H_{15}N_3S$
$M_r = 185.29$
Monoclinic, $P2_1/n$
$a = 12.7584 (8)$ Å
$b = 11.7060 (7)$ Å
$c = 13.3452 (8)$ Å
$\beta = 92.273 (2)°$
$V = 1991.5 (2)$ Å^3
$Z = 8$

$F(000) = 800$
$D_x = 1.236$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2990 reflections
$\theta = 3.9–27.0°$
$\mu = 0.28$ mm^{-1}
$T = 298$ K
Block, white
$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Xcalibur Sapphire3
    diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan
    (SADABS; Bruker, 2004)
$T_{min} = 0.699$, $T_{max} = 0.746$

33823 measured reflections
3912 independent reflections
3464 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.8°$
$h = -15\rightarrow15$
$k = -14\rightarrow14$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.091$
$S = 1.06$
3912 reflections
217 parameters
0 restraints

Hydrogen site location: inferred from
    neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.6361P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.36226 (4)	0.06485 (3)	0.43363 (3)	0.05590 (14)
S1B	0.32888 (3)	0.37480 (3)	1.23730 (3)	0.05222 (13)
N3A	0.47697 (9)	0.25310 (10)	0.65467 (9)	0.0424 (3)
N2B	0.23843 (10)	0.27542 (10)	1.07986 (9)	0.0447 (3)
H2B	0.231543	0.342491	1.054142	0.054*
N2A	0.44552 (10)	0.15830 (10)	0.59824 (8)	0.0432 (3)
H2A	0.455647	0.090225	0.620829	0.052*
N1A	0.38303 (12)	0.28310 (11)	0.48068 (10)	0.0567 (4)
H1A1	0.402306	0.337464	0.520658	0.068*
H1A2	0.353446	0.298699	0.423286	0.068*
N3B	0.19979 (10)	0.18009 (10)	1.02925 (9)	0.0459 (3)
C7B	0.12387 (13)	0.30010 (14)	0.77541 (11)	0.0513 (4)
H7B1	0.054775	0.266491	0.765209	0.062*
H7B2	0.120771	0.377224	0.748874	0.062*
N1B	0.30030 (12)	0.15393 (11)	1.20019 (10)	0.0569 (4)
H1B1	0.278309	0.098724	1.162387	0.068*
H1B2	0.330900	0.139585	1.257387	0.068*
C1A	0.39882 (11)	0.17595 (12)	0.50737 (10)	0.0399 (3)
C2B	0.15849 (11)	0.19368 (12)	0.94109 (10)	0.0410 (3)
C3B	0.11911 (14)	0.08565 (13)	0.89161 (12)	0.0533 (4)
H3B1	0.049944	0.099577	0.861264	0.064*
H3B2	0.112277	0.027142	0.942404	0.064*
C4A	0.57595 (16)	0.11539 (15)	0.89648 (12)	0.0619 (5)
H4A1	0.586940	0.035946	0.914709	0.074*
H4A2	0.643974	0.152500	0.899257	0.074*
C8A	0.54954 (14)	0.34168 (14)	0.79911 (12)	0.0549 (4)
H8A1	0.542756	0.406431	0.753965	0.066*
H8A2	0.622996	0.335077	0.819960	0.066*
C7A	0.48644 (15)	0.36587 (16)	0.89122 (13)	0.0659 (5)
H7A1	0.492016	0.446633	0.906777	0.079*
H7A2	0.413189	0.349641	0.874849	0.079*
C2A	0.51753 (11)	0.23580 (12)	0.74279 (10)	0.0395 (3)
C1B	0.28711 (11)	0.26050 (12)	1.17047 (10)	0.0402 (3)
C5B	0.17991 (16)	0.10414 (16)	0.71256 (14)	0.0659 (5)
H5B1	0.109231	0.092553	0.684959	0.079*
H5B2	0.227671	0.069586	0.666594	0.079*
C4B	0.19057 (15)	0.04172 (15)	0.81164 (14)	0.0630 (5)
H4B1	0.262725	0.047682	0.836836	0.076*
H4B2	0.175657	−0.038576	0.800130	0.076*
C8B	0.15023 (12)	0.30606 (12)	0.88766 (11)	0.0443 (3)
H8B1	0.216397	0.346083	0.897653	0.053*
H8B2	0.096817	0.351409	0.918760	0.053*
C3A	0.53213 (14)	0.11999 (13)	0.78878 (11)	0.0506 (4)
H3A1	0.578569	0.076577	0.747354	0.061*
H3A2	0.464727	0.081536	0.786133	0.061*

C6B	0.20140 (15)	0.23161 (16)	0.71647 (13)	0.0619 (5)
H6B1	0.271208	0.243695	0.746025	0.074*
H6B2	0.200863	0.260753	0.648405	0.074*
C5A	0.50865 (18)	0.17020 (17)	0.97414 (13)	0.0726 (5)
H5A1	0.526310	0.136075	1.038862	0.087*
H5A2	0.435772	0.152300	0.957581	0.087*
C6A	0.51947 (16)	0.29866 (17)	0.98366 (13)	0.0650 (5)
H6A1	0.477872	0.324016	1.038739	0.078*
H6A2	0.592196	0.316471	1.001002	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0894 (3)	0.0358 (2)	0.0411 (2)	−0.00783 (18)	−0.01484 (19)	−0.00011 (15)
S1B	0.0670 (3)	0.0429 (2)	0.0457 (2)	−0.00184 (17)	−0.01074 (18)	−0.00288 (16)
N3A	0.0522 (7)	0.0365 (6)	0.0382 (6)	−0.0023 (5)	−0.0011 (5)	−0.0036 (5)
N2B	0.0599 (7)	0.0347 (6)	0.0388 (6)	0.0003 (5)	−0.0047 (5)	−0.0003 (5)
N2A	0.0606 (7)	0.0334 (6)	0.0351 (6)	0.0012 (5)	−0.0041 (5)	−0.0021 (5)
N1A	0.0874 (10)	0.0363 (6)	0.0451 (7)	0.0066 (6)	−0.0151 (7)	−0.0027 (5)
N3B	0.0592 (7)	0.0351 (6)	0.0429 (6)	−0.0019 (5)	−0.0027 (5)	−0.0015 (5)
C7B	0.0589 (9)	0.0437 (8)	0.0503 (8)	−0.0043 (7)	−0.0118 (7)	0.0072 (7)
N1B	0.0825 (10)	0.0411 (7)	0.0458 (7)	0.0054 (7)	−0.0131 (7)	0.0013 (6)
C1A	0.0468 (7)	0.0375 (7)	0.0355 (7)	0.0004 (6)	0.0023 (5)	−0.0010 (5)
C2B	0.0468 (7)	0.0352 (7)	0.0411 (7)	−0.0018 (6)	0.0018 (6)	−0.0016 (6)
C3B	0.0709 (10)	0.0354 (7)	0.0530 (9)	−0.0098 (7)	−0.0072 (8)	0.0003 (7)
C4A	0.0868 (12)	0.0516 (9)	0.0463 (9)	0.0098 (9)	−0.0095 (8)	0.0046 (7)
C8A	0.0733 (11)	0.0415 (8)	0.0488 (8)	−0.0128 (7)	−0.0122 (8)	−0.0004 (7)
C7A	0.0771 (12)	0.0584 (10)	0.0608 (10)	0.0140 (9)	−0.0154 (9)	−0.0240 (8)
C2A	0.0417 (7)	0.0388 (7)	0.0380 (7)	−0.0023 (6)	0.0020 (5)	−0.0028 (6)
C1B	0.0425 (7)	0.0407 (7)	0.0376 (7)	0.0034 (6)	0.0035 (5)	−0.0002 (6)
C5B	0.0755 (12)	0.0659 (11)	0.0566 (10)	−0.0118 (9)	0.0078 (9)	−0.0245 (9)
C4B	0.0680 (11)	0.0459 (9)	0.0738 (11)	0.0080 (8)	−0.0148 (9)	−0.0209 (8)
C8B	0.0537 (8)	0.0343 (7)	0.0449 (8)	−0.0003 (6)	0.0017 (6)	−0.0022 (6)
C3A	0.0690 (10)	0.0407 (8)	0.0417 (8)	0.0039 (7)	−0.0029 (7)	−0.0030 (6)
C6B	0.0734 (11)	0.0675 (11)	0.0453 (8)	−0.0214 (9)	0.0077 (8)	−0.0101 (8)
C5A	0.0998 (15)	0.0739 (13)	0.0446 (9)	−0.0177 (11)	0.0110 (9)	−0.0009 (9)
C6A	0.0768 (12)	0.0725 (12)	0.0460 (9)	−0.0025 (9)	0.0047 (8)	−0.0177 (8)

Geometric parameters (Å, °)

S1A—C1A	1.6855 (14)	C4A—H4A1	0.9700
S1B—C1B	1.6828 (14)	C4A—H4A2	0.9700
N3A—C2A	1.2820 (18)	C8A—C2A	1.4978 (19)
N3A—N2A	1.3913 (16)	C8A—C7A	1.522 (3)
N2B—C1B	1.3486 (18)	C8A—H8A1	0.9700
N2B—N3B	1.3850 (16)	C8A—H8A2	0.9700
N2B—H2B	0.8600	C7A—C6A	1.509 (3)
N2A—C1A	1.3456 (17)	C7A—H7A1	0.9700

N2A—H2A	0.8600	C7A—H7A2	0.9700
N1A—C1A	1.3173 (18)	C2A—C3A	1.497 (2)
N1A—H1A1	0.8600	C5B—C4B	1.512 (3)
N1A—H1A2	0.8600	C5B—C6B	1.518 (3)
N3B—C2B	1.2798 (18)	C5B—H5B1	0.9700
C7B—C6B	1.517 (2)	C5B—H5B2	0.9700
C7B—C8B	1.524 (2)	C4B—H4B1	0.9700
C7B—H7B1	0.9700	C4B—H4B2	0.9700
C7B—H7B2	0.9700	C8B—H8B1	0.9700
N1B—C1B	1.3178 (19)	C8B—H8B2	0.9700
N1B—H1B1	0.8600	C3A—H3A1	0.9700
N1B—H1B2	0.8600	C3A—H3A2	0.9700
C2B—C8B	1.4981 (19)	C6B—H6B1	0.9700
C2B—C3B	1.5038 (19)	C6B—H6B2	0.9700
C3B—C4B	1.521 (2)	C5A—C6A	1.515 (3)
C3B—H3B1	0.9700	C5A—H5A1	0.9700
C3B—H3B2	0.9700	C5A—H5A2	0.9700
C4A—C5A	1.515 (3)	C6A—H6A1	0.9700
C4A—C3A	1.522 (2)	C6A—H6A2	0.9700
C2A—N3A—N2A	117.89 (12)	H7A1—C7A—H7A2	107.5
C1B—N2B—N3B	118.37 (12)	N3A—C2A—C3A	123.94 (12)
C1B—N2B—H2B	120.8	N3A—C2A—C8A	114.94 (13)
N3B—N2B—H2B	120.8	C3A—C2A—C8A	121.12 (12)
C1A—N2A—N3A	118.25 (11)	N1B—C1B—N2B	116.18 (13)
C1A—N2A—H2A	120.9	N1B—C1B—S1B	124.00 (11)
N3A—N2A—H2A	120.9	N2B—C1B—S1B	119.81 (11)
C1A—N1A—H1A1	120.0	C4B—C5B—C6B	115.80 (14)
C1A—N1A—H1A2	120.0	C4B—C5B—H5B1	108.3
H1A1—N1A—H1A2	120.0	C6B—C5B—H5B1	108.3
C2B—N3B—N2B	118.27 (12)	C4B—C5B—H5B2	108.3
C6B—C7B—C8B	114.26 (13)	C6B—C5B—H5B2	108.3
C6B—C7B—H7B1	108.7	H5B1—C5B—H5B2	107.4
C8B—C7B—H7B1	108.7	C5B—C4B—C3B	114.50 (14)
C6B—C7B—H7B2	108.7	C5B—C4B—H4B1	108.6
C8B—C7B—H7B2	108.7	C3B—C4B—H4B1	108.6
H7B1—C7B—H7B2	107.6	C5B—C4B—H4B2	108.6
C1B—N1B—H1B1	120.0	C3B—C4B—H4B2	108.6
C1B—N1B—H1B2	120.0	H4B1—C4B—H4B2	107.6
H1B1—N1B—H1B2	120.0	C2B—C8B—C7B	115.87 (12)
N1A—C1A—N2A	116.57 (12)	C2B—C8B—H8B1	108.3
N1A—C1A—S1A	122.76 (11)	C7B—C8B—H8B1	108.3
N2A—C1A—S1A	120.67 (10)	C2B—C8B—H8B2	108.3
N3B—C2B—C8B	124.43 (13)	C7B—C8B—H8B2	108.3
N3B—C2B—C3B	114.67 (13)	H8B1—C8B—H8B2	107.4
C8B—C2B—C3B	120.89 (12)	C2A—C3A—C4A	117.02 (13)
C2B—C3B—C4B	113.17 (14)	C2A—C3A—H3A1	108.0
C2B—C3B—H3B1	108.9	C4A—C3A—H3A1	108.0

C4B—C3B—H3B1	108.9	C2A—C3A—H3A2	108.0
C2B—C3B—H3B2	108.9	C4A—C3A—H3A2	108.0
C4B—C3B—H3B2	108.9	H3A1—C3A—H3A2	107.3
H3B1—C3B—H3B2	107.8	C7B—C6B—C5B	114.63 (15)
C5A—C4A—C3A	115.73 (16)	C7B—C6B—H6B1	108.6
C5A—C4A—H4A1	108.3	C5B—C6B—H6B1	108.6
C3A—C4A—H4A1	108.3	C7B—C6B—H6B2	108.6
C5A—C4A—H4A2	108.3	C5B—C6B—H6B2	108.6
C3A—C4A—H4A2	108.3	H6B1—C6B—H6B2	107.6
H4A1—C4A—H4A2	107.4	C4A—C5A—C6A	115.19 (16)
C2A—C8A—C7A	114.62 (14)	C4A—C5A—H5A1	108.5
C2A—C8A—H8A1	108.6	C6A—C5A—H5A1	108.5
C7A—C8A—H8A1	108.6	C4A—C5A—H5A2	108.5
C2A—C8A—H8A2	108.6	C6A—C5A—H5A2	108.5
C7A—C8A—H8A2	108.6	H5A1—C5A—H5A2	107.5
H8A1—C8A—H8A2	107.6	C7A—C6A—C5A	115.30 (15)
C6A—C7A—C8A	115.06 (15)	C7A—C6A—H6A1	108.5
C6A—C7A—H7A1	108.5	C5A—C6A—H6A1	108.5
C8A—C7A—H7A1	108.5	C7A—C6A—H6A2	108.5
C6A—C7A—H7A2	108.5	C5A—C6A—H6A2	108.5
C8A—C7A—H7A2	108.5	H6A1—C6A—H6A2	107.5
C2A—N3A—N2A—C1A	177.23 (13)	N3B—N2B—C1B—S1B	−176.43 (10)
C1B—N2B—N3B—C2B	−176.42 (13)	C6B—C5B—C4B—C3B	58.8 (2)
N3A—N2A—C1A—N1A	−2.5 (2)	C2B—C3B—C4B—C5B	−78.37 (18)
N3A—N2A—C1A—S1A	178.06 (10)	N3B—C2B—C8B—C7B	165.36 (14)
N2B—N3B—C2B—C8B	0.9 (2)	C3B—C2B—C8B—C7B	−13.4 (2)
N2B—N3B—C2B—C3B	179.74 (13)	C6B—C7B—C8B—C2B	−58.26 (18)
N3B—C2B—C3B—C4B	−104.03 (16)	N3A—C2A—C3A—C4A	−176.63 (15)
C8B—C2B—C3B—C4B	74.84 (18)	C8A—C2A—C3A—C4A	2.8 (2)
C2A—C8A—C7A—C6A	80.50 (19)	C5A—C4A—C3A—C2A	62.9 (2)
N2A—N3A—C2A—C3A	−0.6 (2)	C8B—C7B—C6B—C5B	85.86 (19)
N2A—N3A—C2A—C8A	179.98 (12)	C4B—C5B—C6B—C7B	−65.3 (2)
C7A—C8A—C2A—N3A	113.48 (16)	C3A—C4A—C5A—C6A	−82.1 (2)
C7A—C8A—C2A—C3A	−66.0 (2)	C8A—C7A—C6A—C5A	−62.0 (2)
N3B—N2B—C1B—N1B	4.7 (2)	C4A—C5A—C6A—C7A	62.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N1*A*—H1*A*1···N3*A*	0.86	2.22	2.5943 (2)	106
N1*B*—H1*B*1···N3*B*	0.86	2.22	2.5904 (2)	106
N1*A*—H1*A*2···S1*B*[i]	0.86	2.64	3.4642 (2)	160
N1*B*—H1*B*2···S1*A*[ii]	0.86	2.53	3.3499 (2)	161
N2*B*—H2*B*···S1*A*[iii]	0.86	2.87	3.6254 (2)	147

Symmetry codes: (i) $x, y, z−1$; (ii) $x, y, z+1$; (iii) $−x+1/2, y+1/2, −z+3/2$.