5-Amino-1H-benzimidazole-2(3H)-thione: molecular, crystal structure and Hirshfeld surface analysis

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The title compound, C7H7N3S, which has potential biological activity, can be used as a ligand in metal complexation. This compound exists as the thione tautomer in the crystal phase, which is confirmed by the study of its molecular structure. The amino group has pyramidal configuration. In the crystal phase, the two independent molecules in the asymmetric unit form tetramers as a result of N—H/C1/C1/C1S hydrogen bonds. These tetramers are linked by N—H/C1/C1/C1N hydrogen bonds, forming chains/tubes in the [010] direction. The Hirshfeld surface analysis showed that the highest contribution to the total surface is provided by H/C1/C1/C1H interactions as well as S/C1/C1/C1H/H/C1/C1/C1C contacts associated with X—H/C1/C1/S hydrogen bonds and X—H/C1/C1/C1C(π) interactions.

1. Chemical context

Benzimidazoles belong to an important class of heterocyclic compounds because of their wide spectra of biological activity. In particular, benzimidazole derivatives are known to possess antibacterial (Chkirate et al., 2020), antimicrobial (Alam et al., 2014), antitumor (Kharitonova et al., 2018; Galal et al., 2010), anti-inflammatory (Rathore et al., 2017), antioxidant (Anastassova et al., 2017), anthelmintic (Kenchappa et al., 2017), antifungal and cytotoxic (Leila et al., 2019) activity. They are also important as starting materials for terminal alkyl cyclotrimerization reactions (Xi et al., 2013) and are used as highly active catalysts for ethylene oligomerization (Haghverdi et al., 2018). The synthesis of 2-amino-1,3-benzimidazole-2-thione has been reported, prepared by first treating o-phenylenediamine CS2 in the presence of KOH under microwave irradiation to give the intermediate 1,3-benzimidazole-2-thione. Nitration of the intermediate followed by reduction of the nitro group with iron powder and concentrated hydrochloric acid gave 2-amino-1,3-benzimidazole-2-thione in a moderately good yield (Samanta et al., 2013; Ahamed et al., 2013). Taking into account the possible biological activity of the obtained compound, it is important to study its molecular and crystal structures.

2. Structural commentary

Two independent molecules (A and B) comprise the asymmetric unit of the title compound (Fig. 1). The molecules
slightly differ from each other in their degree of planarity: all non-hydrogen atoms lie in the same plane with an accuracy of 0.05 Å in molecule A and with an accuracy of 0.02 Å in molecule B. Analysis of the molecular structure revealed that the C=S tautomer is found in the crystal, as confirmed by the length of the C7—S1 bond [1.687 (3) Å in molecule A and 1.684 (3) Å in molecule B], the equal lengths of the C7—N1 and C7—N2 bonds [1.345 (3) and 1.347 (3) Å in molecule A and 1.351 (3) and 1.349 (3) Å in molecule B] and the localization of hydrogen atoms at all the nitrogen atoms from the electron-density difference maps. The amino groups in both molecules are pyramidal, the sum of the bond angles centered at the nitrogen atom is 331.5° in molecule A and 340.9° in molecule B.

3. Supramolecular features

In the crystal, the molecules form tetramers as a result of the N2A—H2NA···S1B and N2B—H2NB···S1A hydrogen bonds (Fig. 2, Table 1). The tetramers are linked by N1A···H1NA···N3B and N1B—H1NB···N3A hydrogen bonds, forming a tube in the [010] direction (Figs. 3 and 4). Adjacent tubes are connected by weaker N—H···C(π), C—H···N—H···S and C—H···C(π) interactions (Table 1).

4. Hirshfeld surface analysis

One of the modern methods for analysing intermolecular interactions is Hirshfeld surface analysis (Spackman & Jaya-

### Table 1

|        | D—H ·· A | D—H ·· A | D···A | D—H ·· A |
|--------|----------|----------|-------|----------|
| N1A—H1NA···N3B | 0.80 (3) | 2.06 (3) | 2.856 (3) | 176 (3) |
| N2A—H2NA···S1B | 0.82 (3) | 2.54 (3) | 3.295 (2) | 154 (3) |
| N3A—H3NA···S1A | 0.84 (4) | 2.75 (4) | 3.551 (3) | 159 (3) |
| N3A—H3NB···C4B | 0.89 (4) | 2.71 (4) | 3.483 (4) | 145 (3) |
| N3A—H3NB···CSB | 0.89 (4) | 2.81 (4) | 3.645 (4) | 155 (3) |
| N1B—H1NB···N3A | 0.88 (3) | 2.02 (3) | 2.884 (3) | 171 (3) |
| N2B—H2NB···S1A | 0.85 (3) | 2.56 (3) | 3.340 (2) | 153 (3) |
| N3B—H3NC···S1B | 0.86 (3) | 2.91 (3) | 3.672 (3) | 149 (2) |
| N3B—H3ND···S1B | 0.85 (3) | 2.70 (3) | 3.477 (3) | 153 (3) |
| C5A—H5A···S1A | 0.96 (3) | 2.96 (3) | 3.656 (3) | 130.2 (19) |
| C5B—H5B···CLA | 0.90 (3) | 2.78 (3) | 3.562 (3) | 147 (3) |

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

Figure 1

Molecular structures of molecules A and B showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Figure 2

Tetramer of molecules A and B formed by N2A—H2NA···S1B and N2B—H2NB···S1A hydrogen bonds.

Figure 3

Chain/tube of tetramers linked by N1A···H1NA···N3B and N1B—H1NB···N3A hydrogen bonds.
Analysis of the fingerprint plots showed the presence of strong intermolecular interactions indicated as sharp spikes (Fig. 6a, 6b). The most significant contribution to the total Hirshfeld surface is provided by H⋯H interactions in both molecules (Fig. 6c, 6g). The contributions of S⋯H/H⋯S and C⋯H/H⋯C interactions associated with X—H⋯S and X—H⋯C (π) hydrogen bonds are similar (Fig. 6d–i). Surprisingly, the contribution of N⋯H/H⋯N interactions proved to be the lowest (Fig. 6f, 6j). It may be explained by the participation of the nitrogen lone pair in hydrogen bonding as a proton acceptor.

5. Database survey
A search of the Cambridge Structural Database (Version 5.42, update of November 2020; Groom et al., 2016) revealed the structure of the monohydrate of the title compound (ODAXID; Hadjikakou & Light, 2016). It should be noted that the amino group was refined as planar in this structure. However, analysis of the intermolecular interactions showed that this amino group participates in a hydrogen bond with the hydrate water molecule as a proton acceptor. Such a hydrogen bonding has to result in pyramidalization of the amino group. To check this presumption, we have optimized the ODAXID structure with a periodic boundary using the PBE functional (Adamo & Barone, 1999) within Quantum Espresso (Gianozzi et al., 2009, 2017). The unit-cell parameters were fixed while the molecular structures of both molecules found in the asymmetric unit were optimized. The result of this optimization shows that the amino group has to be pyramidal (Fig. 7).

6. Crystallization
5-Amino-1H-benzimidazole-2(3H)-thione was purchased from Sigma-Aldrich for use as a ligand in complexation with metals. The reaction of the title compound with nickel acetate in an aqueous alcoholic medium did not result in complex formation. The formed colourless needle-like crystals proved to be anhydrous form of the ligand with $T_{\text{melt}} = 513–517$ K.

7. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2. All the hydrogen atoms were located in difference-Fourier maps and refined using an isotropic approximation.
Table 2
Experimental details.

| Crystal data          | Value          |
|-----------------------|---------------|
| Chemical formula      | C₇H₇N₃S      |
| Mᵣ                   | 165.22        |
| Crystal system, space group | Monoclinic, C2/c |
| Temperature (K)       | 293           |
| No. of measured, independent and observed reflections | 12390, 2787, 2417 |
| R[F² > 2σ(F²)]        | 0.052, 0.138, 1.05 |
| No. of reflections    | 2787          |
| H-atom treatment      | All H-atom parameters refined |
| Δρmax, Δρmin (e Å⁻³) | 0.33, -0.27 |

Data collection
Diffractometer        Xcalibur, Sapphire3
Absorption correction  Multi-scan (CrysAlis PRO; Rigaku OD, 2018)
Tmin, Tmax             0.370, 1.000
No. of measured, independent and observed reflections | 12390, 2787, 2417 |

Refinement
H-atom treatment      All H-atom parameters refined

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supporting information

5-Amino-1H-benzimidazole-2(3H)-thione: molecular, crystal structure and Hirshfeld surface analysis

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Computing details

Data collection: CrysAlis PRO (Rigaku OD, 2018); cell refinement: CrysAlis PRO (Rigaku OD, 2018); data reduction: CrysAlis PRO (Rigaku OD, 2018); program(s) used to solve structure: SHELXT2014/5 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2016/6 (Sheldrick, 2015b); molecular graphics: Mercury (Macrae et al., 2020); software used to prepare material for publication: Olex2 (Dolomanov et al., 2009).

5-Amino-1H-benzimidazole-2(3H)-thione

Crystal data

C7H7N3S

Mr = 165.22

Monoclinic, C2/c

a = 16.1179 (14) Å

b = 11.8796 (11) Å

c = 16.5649 (15) Å

β = 91.974 (8)°

V = 3169.9 (5) Å3

Z = 16

F(000) = 1376

Dx = 1.385 Mg m−3

Mo Ka radiation, λ = 0.71073 Å

Cell parameters from 2937 reflections

θ = 3.5–26.9°

µ = 0.34 mm−1

T = 293 K

Plate, colorless

0.80 × 0.26 × 0.08 mm

Data collection

Xcalibur, Sapphire3
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Detector resolution: 16.1827 pixels mm−1

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2018)

T_{min} = 0.370, T_{max} = 1.000

12390 measured reflections

2787 independent reflections

2417 reflections with I > 2σ(I)

R_{int} = 0.079

θ_{max} = 25.0°, θ_{min} = 3.2°

h = −19→18

k = −14→14

l = −19→19

Refinement

Refinement on F^2

Least-squares matrix: full

R[F^2 > 2σ(F^2)] = 0.052

wR(F^2) = 0.138

S = 1.05

2787 reflections

255 parameters

0 restraints

Hydrogen site location: difference Fourier map

All H-atom parameters refined

w = 1/[σ^2(Fo^2) + (0.0719P)^2 + 1.8442P]

where P = (Fo^2 + 2Fc^2)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.33 e Å^{-3}

Δρ_{min} = −0.27 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)**

| Atom | x   | y   | z   | Uiso* |
|------|-----|-----|-----|-------|
| S1B  | 0.37352 (5) | 0.24474 (6) | 0.14471 (5) | 0.0546 (3) |
| N1B  | 0.44866 (14) | 0.44339 (17) | 0.11231 (14) | 0.0388 (5) |
| H1NB | 0.402 (2) | 0.477 (3) | 0.098 (2) | 0.060 (9)* |
| N2B  | 0.53394 (13) | 0.31429 (19) | 0.15625 (14) | 0.0406 (5) |
| H2NB | 0.5498 (18) | 0.248 (2) | 0.1694 (18) | 0.048 (8)* |
| N3B  | 0.66860 (17) | 0.7248 (2) | 0.07344 (15) | 0.0425 (6) |
| H3NC | 0.6461 (19) | 0.754 (2) | 0.031 (2) | 0.047 (9)* |
| H3ND | 0.721 (2) | 0.729 (2) | 0.0726 (18) | 0.049 (9)* |
| C1B  | 0.52713 (14) | 0.4917 (2) | 0.11265 (14) | 0.0345 (6) |
| C2B  | 0.55387 (16) | 0.5967 (2) | 0.08966 (15) | 0.0365 (6) |
| H2B  | 0.5159 (17) | 0.655 (2) | 0.0704 (16) | 0.049 (8)* |
| C3B  | 0.63884 (15) | 0.6175 (2) | 0.09525 (14) | 0.0360 (6) |
| C4B  | 0.69331 (17) | 0.5355 (2) | 0.12677 (17) | 0.0428 (6) |
| H4B  | 0.748 (2) | 0.556 (2) | 0.1314 (18) | 0.051 (8)* |
| C5B  | 0.66596 (17) | 0.4308 (2) | 0.15038 (18) | 0.0449 (7) |
| H5B  | 0.699 (2) | 0.378 (3) | 0.174 (2) | 0.063 (9)* |
| C6B  | 0.58190 (15) | 0.4093 (2) | 0.14187 (15) | 0.0365 (6) |
| C7B  | 0.45329 (16) | 0.3353 (2) | 0.13759 (15) | 0.0382 (6) |
| S1A  | 0.60205 (5) | 1.05022 (6) | 0.13822 (4) | 0.0479 (3) |
| N1A  | 0.63692 (14) | 0.85370 (18) | 0.21461 (13) | 0.0397 (5) |
| H1NA | 0.6481 (17) | 0.819 (3) | 0.1755 (18) | 0.044 (8)* |
| N2A  | 0.59495 (13) | 0.9834 (2) | 0.29505 (13) | 0.0383 (5) |
| H2NA | 0.5855 (18) | 1.049 (3) | 0.3087 (18) | 0.046 (8)* |
| N3A  | 0.69384 (16) | 0.57892 (19) | 0.43321 (16) | 0.0420 (6) |
| H3NA | 0.737 (2) | 0.556 (3) | 0.411 (2) | 0.061 (11)* |
| H3NB | 0.705 (2) | 0.580 (3) | 0.486 (2) | 0.067 (10)* |
| C1A  | 0.63986 (15) | 0.8070 (2) | 0.29109 (14) | 0.0343 (6) |
| C2A  | 0.66733 (16) | 0.7028 (2) | 0.31939 (16) | 0.0382 (6) |
| H2A  | 0.6856 (16) | 0.644 (2) | 0.2830 (17) | 0.044 (7)* |
| C3A  | 0.66781 (15) | 0.6855 (2) | 0.40200 (15) | 0.0354 (6) |
| C4A  | 0.63934 (17) | 0.7692 (2) | 0.45370 (17) | 0.0421 (6) |
| H4A  | 0.6398 (18) | 0.753 (2) | 0.5104 (19) | 0.050 (8)* |
| C5A  | 0.61082 (18) | 0.8722 (2) | 0.42509 (16) | 0.0432 (6) |
| H5A  | 0.5872 (16) | 0.927 (2) | 0.4604 (16) | 0.039 (7)* |
| C6A  | 0.61262 (15) | 0.8897 (2) | 0.34291 (15) | 0.0344 (5) |
| C7A  | 0.61113 (15) | 0.9613 (2) | 0.21741 (15) | 0.0373 (6) |
Atomic displacement parameters (Å²)

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| S1B | 0.0502 (5)  | 0.0400 (4)  | 0.0723 (6)  | −0.0110 (3) | −0.0143 (4) | 0.0145 (3)  |
| N1B | 0.0347 (12) | 0.0318 (11) | 0.0493 (13) | 0.0011 (9)  | −0.0089 (10)| 0.0041 (10) |
| N2B | 0.0421 (12) | 0.0278 (12) | 0.0514 (13) | 0.0040 (9)  | −0.0072 (10)| 0.0060 (10) |
| N3B | 0.0432 (14) | 0.0435 (14) | 0.0408 (13) | −0.0074 (11)| 0.0015 (11) | 0.0010 (11) |
| C1B | 0.0343 (13) | 0.0337 (13) | 0.0350 (12) | 0.0000 (10) | −0.0058 (10)| −0.0007 (10)|
| C2B | 0.0388 (14) | 0.0304 (13) | 0.0399 (13) | 0.0032 (11) | −0.0035 (11)| 0.0005 (11) |
| C3B | 0.0421 (14) | 0.0340 (13) | 0.0320 (12) | −0.0014 (11)| 0.0004 (11) | −0.0065 (10)|
| C4B | 0.0343 (14) | 0.0460 (16) | 0.0477 (15) | 0.0099 (12) | −0.0031 (12)| −0.0043 (12)|
| C5B | 0.0383 (15) | 0.0410 (15) | 0.0546 (16) | 0.0082 (12) | −0.0109 (13)| 0.0001 (13) |
| C6B | 0.0379 (13) | 0.0321 (13) | 0.0391 (13) | 0.0036 (11) | −0.0056 (11)| 0.0005 (11) |
| C7B | 0.0439 (14) | 0.0322 (13) | 0.0379 (13) | −0.0004 (11)| −0.0069 (11)| 0.0027 (11) |
| S1A | 0.0595 (5)  | 0.0385 (4)  | 0.0459 (4)  | 0.0055 (3)  | 0.0033 (3)  | 0.0090 (3)  |
| N1A | 0.0565 (14) | 0.0307 (12) | 0.0322 (11) | 0.0023 (10) | 0.0034 (10) | −0.0023 (10)|
| N2A | 0.0462 (13) | 0.0302 (12) | 0.0384 (12) | 0.0063 (10) | 0.0006 (10) | −0.0047 (10)|
| N3A | 0.0443 (14) | 0.0378 (13) | 0.0432 (13) | −0.0024 (10)| −0.0074 (12)| 0.0044 (11) |
| C1A | 0.0376 (13) | 0.0309 (13) | 0.0342 (12) | −0.0024 (10)| −0.0023 (10)| −0.0008 (10)|
| C2A | 0.0455 (15) | 0.0297 (13) | 0.0392 (14) | −0.0013 (11)| −0.0011 (11)| −0.0038 (11)|
| C3A | 0.0358 (13) | 0.0318 (13) | 0.0385 (13) | −0.0060 (10)| −0.0054 (10)| 0.0000 (11) |
| C4A | 0.0474 (15) | 0.0447 (15) | 0.0338 (14) | −0.0055 (12)| −0.0048 (12)| 0.0008 (12) |
| C5A | 0.0542 (16) | 0.0397 (15) | 0.0354 (14) | 0.0016 (12) | −0.0008 (12)| −0.0068 (12)|
| C6A | 0.0358 (13) | 0.0305 (13) | 0.0368 (13) | 0.0002 (10) | −0.0024 (10)| −0.0014 (10)|
| C7A | 0.0355 (13) | 0.0330 (13) | 0.0430 (15) | −0.0003 (10)| −0.0017 (11)| −0.0011 (11)|

Geometric parameters (Å, °)

|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| S1B—C7B | 1.684 (3) | S1A—C7A | 1.686 (3) |
| N1B—C7B | 1.351 (3) | N1A—C7A | 1.346 (3) |
| N1B—C1B | 1.389 (3) | N1A—C1A | 1.382 (3) |
| N1B—H1NB | 0.88 (3) | N1A—H1NA | 0.80 (3) |
| N2B—C7B | 1.349 (3) | N2A—C7A | 1.347 (3) |
| N2B—C6B | 1.393 (3) | N2A—C6A | 1.390 (3) |
| N2B—H2NB | 0.85 (3) | N2A—H2NA | 0.82 (3) |
| N3B—C3B | 1.413 (3) | N3A—C3A | 1.426 (3) |
| N3B—H3NC | 0.86 (3) | N3A—H3NA | 0.84 (4) |
| N3B—H3ND | 0.85 (3) | N3A—H3NB | 0.89 (4) |
| C1B—C2B | 1.378 (4) | C1A—C6A | 1.386 (3) |
| C1B—C6B | 1.394 (3) | C1A—C2A | 1.390 (4) |
| C2B—C3B | 1.391 (4) | C2A—C3A | 1.384 (3) |
| C2B—H2B | 0.97 (3) | C2A—H2A | 0.98 (3) |
| C3B—C4B | 1.401 (4) | C3A—C4A | 1.400 (4) |
| C4B—C5B | 1.380 (4) | C4A—C5A | 1.385 (4) |
| C4B—H4B | 0.92 (3) | C4A—H4A | 0.96 (3) |
| C5B—C6B | 1.381 (4) | C5A—C6A | 1.378 (4) |
| C5B—H5B | 0.90 (3) | C5A—H5A | 0.96 (3) |
C7B—N1B—C1B 110.5 (2) C7A—N1A—C1A 110.5 (2)
C7B—N1B—H1NB 124 (2) C7A—N1A—H1NA 127 (2)
C1B—N1B—H1NB 125 (2) C1A—N1A—H1NA 122 (2)
C7B—N2B—C6B 110.3 (2) C7A—N2A—C6A 110.3 (2)
C7B—N2B—H2NB 121 (2) C7A—N2A—H2NA 119 (2)
C6B—N2B—H2NB 129 (2) C6A—N2A—H2NA 129 (2)
C3B—N3B—H3NC 116 (2) C3A—N3A—H3NA 111 (2)
C3B—N3B—H3ND 114 (2) C3A—N3A—H3NB 113 (2)
H3NC—N3B—H3ND 111 (3) H3NA—N3A—H3NB 108 (3)
C2B—C1B—N1B 131.8 (2) N1A—C1A—C6A 106.3 (2)
C2B—C1B—C6B 122.1 (2) N1A—C1A—C2A 131.8 (2)
N1B—C1B—C6B 106.1 (2) C6A—C1A—C2A 121.8 (2)
C1B—C2B—C3B 117.3 (2) C3A—C2A—C1A 117.2 (2)
C1B—C2B—H2B 122.3 (17) C3A—C2A—H2A 120.9 (16)
C2B—C3B—H4B 122.1 (18) C5A—C4A—C3A 122.0 (2)
C2B—C3B—N3B 119.0 (2) C2A—C3A—N3A 118.2 (2)
C2B—C3B—H2B 119 (2) C4A—C3A—N3A 120.5 (2)
C5B—C4B—C3B 120.6 (2) C5A—C4A—C3A 120.0 (3)
C5B—C4B—H4B 115.9 (18) C3A—C4A—H4A 118.0 (17)
C4B—C5B—C6B 117.4 (3) C6A—C5A—C4A 117.0 (3)
C4B—C5B—H5B 124 (2) C6A—C5A—H5A 121.3 (16)
C6B—C5B—H5B 119 (2) C4A—C5A—H5A 121.6 (16)
C5B—C6B—N2B 132.9 (2) C5A—C6A—C1A 121.5 (2)
C5B—C6B—C1B 112.8 (2) C5A—C6A—N2A 123.2 (2)
N2B—C6B—C1B 106.3 (2) C1A—C6A—N2A 106.1 (2)
N2B—C7B—N1B 106.8 (2) C1A—C7A—C6A 106.7 (2)
N2B—C7B—S1B 126.69 (19) N1A—C7A—S1A 125.9 (2)
N1B—C7B—S1B 126.5 (2) N2A—C7A—S1A 127.3 (2)
C7B—N1B—C1B—C2B 177.4 (3) C7A—N1A—C1A—C6A 1.4 (3)
C7B—N1B—C1B—C6B −1.7 (3) C7A—N1A—C1A—C2A −175.1 (3)
N1B—C1B—C2B—C3B −177.8 (2) N1A—C1A—C2A—C3A 174.9 (3)
C6B—C1B—C2B—C3B 1.2 (4) C6A—C1A—C2A—C3A −1.1 (4)
C1B—C2B—C3B—C4B −2.9 (4) C1A—C2A—C3A—C4A 1.8 (4)
C1B—C2B—C3B—N3B −179.0 (2) C1A—C2A—C3A—N3A 178.6 (2)
C2B—C3B—C4B—C5B 2.4 (4) C2A—C3A—C4A—C5A −0.8 (4)
N3B—C3B—C4B—C5B 178.5 (3) N3A—C3A—C4A—C5A −177.6 (2)
C3B—C4B—C5B—C6B 0.0 (4) C3A—C4A—C5A—C6A −0.8 (4)
C4B—C5B—C6B—N2B 177.3 (3) C4A—C5A—C6A—C1A 1.5 (4)
C4B—C5B—C6B—C1B −1.8 (4) C4A—C5A—C6A—N2A −174.7 (3)
C7B—N2B—C6B—C5B −179.4 (3) N1A—C1A—C6A—C5A −177.5 (2)
C7B—N2B—C6B—C1B −0.3 (3) C2A—C1A—C6A—C5A −0.6 (4)
C2B—C1B—C6B—C5B 1.2 (4) N1A—C1A—C6A—N2A −0.4 (3)
C2B—C1B—C6B—N2B −179.6 (2) C2A—C1A—C6A—N2A 176.5 (2)
C2B—C1B—C6B—N2B −178.1 (2) C7A—N2A—C6A—C5A 176.0 (3)
N1B—C1B—C6B—N2B 1.2 (3) C7A—N2A—C6A—C1A −0.7 (3)

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sup-4
### Hydrogen-bond geometry (Å, °)

| D—H···A     | D—H  | H···A | D···A  | D—H···A |
|------------|------|------|-------|---------|
| N1A···N3B  | 0.80 | 2.06 | 2.856 | 176     |
| N2A···S1B  | 0.82 | 2.54 | 3.295 | 154     |
| N3A···C4B  | 0.89 | 2.71 | 3.483 | 145     |
| N3A···S1A  | 0.89 | 2.81 | 3.643 | 155     |
| N1B···N3A  | 0.88 | 2.02 | 2.884 | 171     |
| N2B···S1A  | 0.85 | 2.56 | 3.340 | 153     |
| N3B···S1B  | 0.86 | 2.91 | 3.672 | 149     |
| N3B···S1B  | 0.85 | 2.70 | 3.477 | 153     |
| C5A···S1A  | 0.96 | 2.96 | 3.656 | 130.2   |
| C5B···C1A  | 0.90 | 2.78 | 3.562 | 147     |

Symmetry codes: (i) −x+1, y+1, −z+1/2; (ii) −x+3/2, y−1/2, −z+1/2; (iii) x, −y+1, z+1/2; (iv) −x+1, y, −z+1/2; (v) x, y−1, z; (vi) −x+1, −y+1, −z; (vii) x+1/2, y+1/2, z; (viii) x, −y+2, z+1/2;