Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

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

Dilnoza Rakhmonova,[a]* Lobar Gapurova,[a] Surayyo Razzoqova,[a] Shakhnoza Kadirova,[a] Batirbay Torambetov,[a] Zukhra Kadirova[a,b] and Svitlana Shishkina[c]

[a]National University of Uzbekistan named after Mirzo Ulugbek, 4 University St, Tashkent, 100174, Uzbekistan, [b]Uzbekistan–Japan Innovation Center of Youth, University Street 2B, 100095, Tashkent, Uzbekistan, and [c]State Scientific Institution "Institute for Single Crystals" of National Academy of Sciences of Ukraine, 60 Nauky ave., 61001 Kharkiv, Ukraine. *Correspondence e-mail: d.rakhmonova81@mail.ru

Received 3 November 2021
Accepted 23 January 2022

Edited by J. Ellena, Universidade de São Paulo, Brazil

Keywords: molecular structure; crystal structure; 5-amino-1*H*-benzimidazole-2(3*H*)-thione; hydrogen bond; Hirshfeld analysis; periodic calculations.

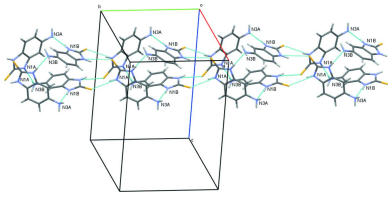
CCDC reference: 2143895

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $C_7H_7N_3S$, 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···S hydrogen bonds. These tetramers are linked by N—H···N 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···H interactions as well as S···H/H···S and C···H/H···C contacts associated with *X*—H···S hydrogen bonds and *X*—H···C(π) interactions.

1. Chemical context

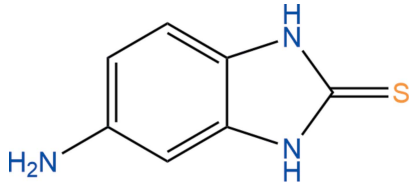
Benzimidazoles belong to an important class of heterocyclic compounds because of their wide spectra of biological activity. In particular, benzimidazole derivatives are known to possess antibacterial (Chkirate *et al.*, 2020), antimicrobial (Alam *et al.*, 2014), antitumor (Kharitonova *et al.*, 2018; 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 alkyne 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 CS_2 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 N2*A*—H2*NA*···S1*B* and N2*B*—H2*NB*···S1*A* hydrogen bonds (Fig. 2, Table 1). The tetramers are linked by N1*A*···H1*NA*—N3*B* and N1*B*—H1*NB*···N3*A* 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···S, 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 & Jayatilaka, 2009; Turner *et al.*, 2017), which allows analysis of the interactions between molecules in a quantitative manner. The Hirshfeld surfaces of molecules *A* and *B* mapped over d_{norm} proved to be very similar (Fig. 5). The red spots indicating strong interactions are found at both hydrogen atoms of the NH fragments as well as in the area of the nitrogen lone pair of the amino group. In addition, red spots are seen at the sulfur atom.

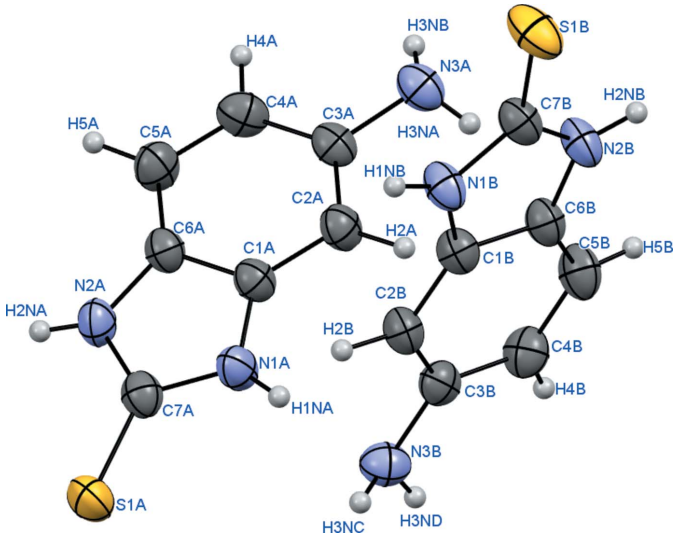


Figure 1
Molecular structures of molecules *A* and *B* showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*NA*···N3*B*	0.80 (3)	2.06 (3)	2.856 (3)	176 (3)
N2*A*—H2*NA*···S1*B*^{i}	0.82 (3)	2.54 (3)	3.295 (2)	154 (3)
N3*A*—H3*NA*···S1*A*^{ii}	0.84 (4)	2.75 (4)	3.551 (3)	159 (3)
N3*A*—H3*NB*···C4*B*^{iii}	0.89 (4)	2.71 (4)	3.483 (4)	145 (3)
N3*A*—H3*NB*···C5*B*^{iii}	0.89 (4)	2.81 (4)	3.643 (4)	155 (3)
N1*B*—H1*NB*···N3*A*^{iv}	0.88 (3)	2.02 (3)	2.884 (3)	171 (3)
N2*B*—H2*NB*···S1*A*^{v}	0.85 (3)	2.56 (3)	3.340 (2)	153 (3)
N3*B*—H3*NC*···S1*B*^{vi}	0.86 (3)	2.91 (3)	3.672 (3)	149 (2)
N3*B*—H3*ND*···S1*B*^{vii}	0.85 (3)	2.70 (3)	3.477 (3)	153 (3)
C5*A*—H5*A*···S1*A*^{viii}	0.96 (3)	2.96 (3)	3.656 (3)	130.2 (19)
C5*B*—H5*B*···C1*A*^{ii}	0.90 (3)	2.78 (3)	3.562 (4)	147 (3)

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

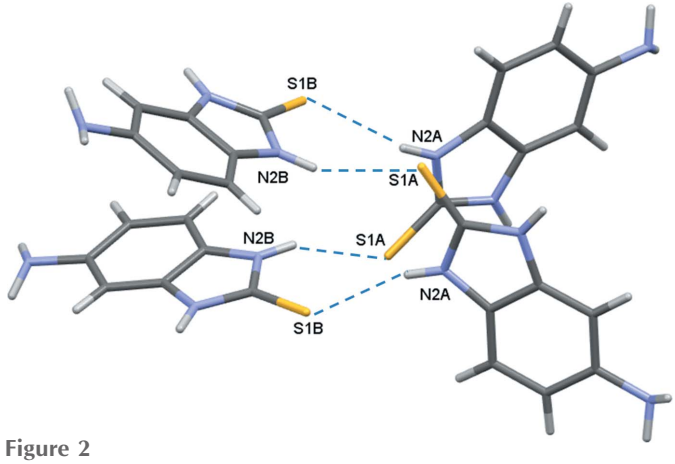


Figure 2
Tetramer of molecules *A* and *B* formed by N2*A*—H2*NA*···S1*B* and N2*B*—H2*NB*···S1*A* hydrogen bonds.

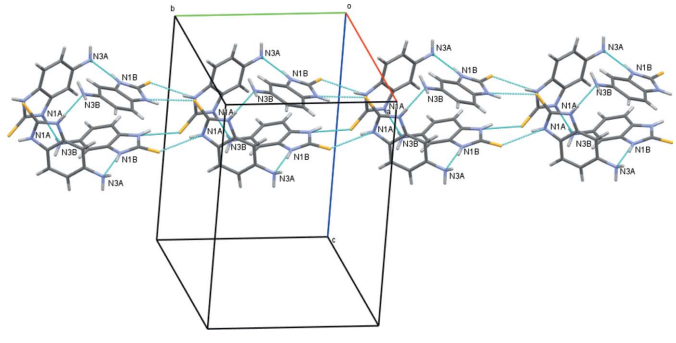


Figure 3
Chain/tube of tetramers linked by N1*A*···H1*NA*—N3*B* and N1*B*—H1*NB*···N3*A* hydrogen bonds.

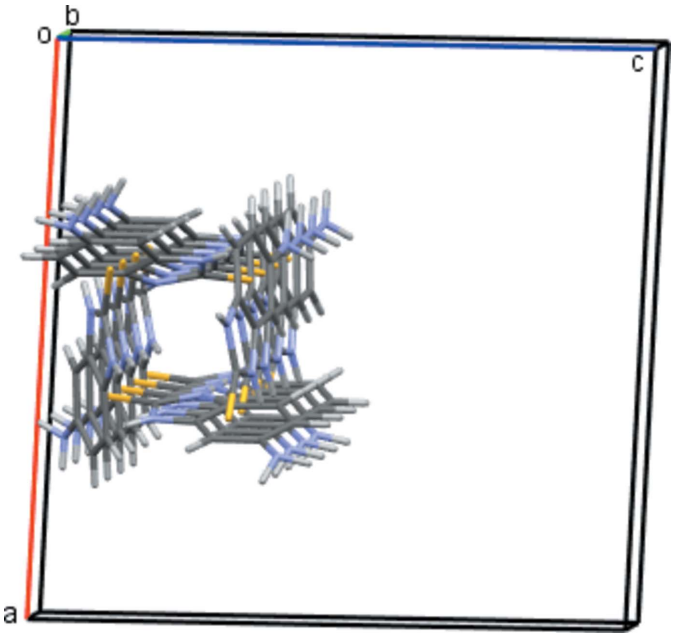


Figure 4
Projection of a tube in the *b*-axis direction.

Analysis of the fingerprint plots showed the presence of strong intermolecular interactions indicated as sharp spikes (Fig. 6*a*, 6*b*). The most significant contribution to the total Hirshfeld surface is provided by H···H interactions in both molecules (Fig. 6*c*, 6*g*). 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. 6*d–i*). Surprisingly, the contribution of N···H/H···N interactions proved to be the lowest (Fig. 6*f*, 6*j*). 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

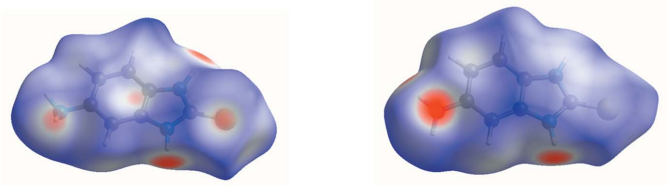


Figure 5
Hirshfeld surfaces mapped over d_{norm} calculated for molecules *A* and *B*.

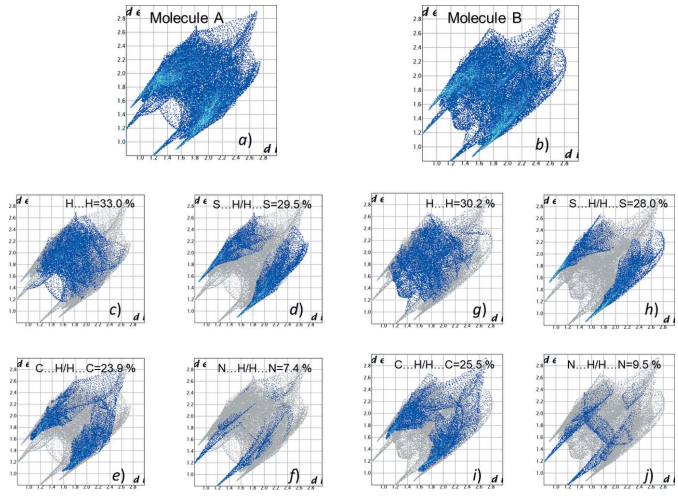


Figure 6
Two-dimensional Hirshfeld fingerprint plot of all contacts for molecules *A* (*a*) and *B* (*b*) and those delineated into H···H (*c*, *g*), S···H/H···S (*d*, *h*), C···H/H···C (*e*, *i*) and N···H/H···N (*f*, *j*) contacts.

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* (Giannozzi *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-1*H*-benzimidazole-2(3*H*)-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 $T_{melt.}$ = 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.

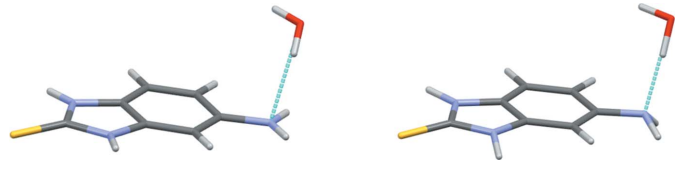


Figure 7
Configuration of the amino group in the structure of ODAXID calculated from the experimental data (Hadjikakou & Light, 2016) and obtained after optimization with a periodic boundary.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_7N_3S$
M_r	165.22
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	16.1179 (14), 11.8796 (11), 16.5649 (15)
β (°)	91.974 (8)
V (Å^3)	3169.9 (5)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.34
Crystal size (mm)	0.80 × 0.26 × 0.08
Data collection	
Diffractometer	Xcalibur, Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.370, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12390, 2787, 2417
R_{int}	0.079
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.138, 1.05
No. of reflections	2787
No. of parameters	255
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.27

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *Olex2* (Dolomanov *et al.*, 2009).

References

Adamo, C. & Barone, V. (1999). *J. Chem. Phys.* **110**, 6158–6170.

Ahamed, M. R., Narren, S. F. & Sadiq, A. S. (2013). *J. Al-Nahrain Uni.* **16**, 77–83.

Alam, F., Dey, B. K., Sharma, K., Chakraborty, A. & Kalita, P. (2014). *Int. J. Drug Res. Tech.* **4**(3), 31–38.

Anastassova, N., Mavrova, A., Yancheva, D., Kondeva-Burdina, M., Tzankova, V., Stoyanov, S., Shivachev, B. L. & Nikolova, R. P. (2017). *Arab. J. Chem.* **11**, 353–369.

Chkirate, K., Karrouchi, K., Dege, N., Sebbar, N. K., Ejjoummany, A., Radi, S., Adarsh, N. N., Talbaoui, A., Ferbinteanu, M., Essassi, E. M. & Garcia, Y. (2020). *New J. Chem.* **44**, 2210–2221.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Galal, S. A., Hegab, K. H., Hashem, A. M. & Youssef, N. S. (2010). *Eur. J. Med. Chem.* **45**, 5685–5691.

Giannozzi, P., Andreussi, O., Brumme, T., Bunau, O., Buongiorno Nardelli, M., Calandra, M., Car, R., Cavazzoni, C., Ceresoli, D., Cococcioni, M., Colonna, N., Carnimeo, I., Dal Corso, A., de Gironcoli, S., Delugas, P., DiStasio, R. A., Ferretti, A., Floris, A., Fratesi, G., Fugallo, G., Gebauer, R., Gerstmann, U., Giustino, F., Gorni, T., Jia, J., Kawamura, M., Ko, H. Y., Kokalj, A., Küçükbenli, E., Lazzeri, M., Marsili, M., Marzari, N., Mauri, F., Nguyen, N. L., Nguyen, H. V., Otero-de-la-Roza, A., Paulatto, L., Poncé, S., Rocca, D., Sabatini, R., Santra, B., Schlipf, M., Seitsonen, A. P., Smogunov, A., Timrov, I., Thonhauser, T., Umari, P., Vast, N., Wu, X. & Baroni, S. (2017). *J. Phys. Condens. Matter*, **29**, 465901.

Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R., Cavazzoni, C., Ceresoli, D., Chiarotti, G. L., Cococcioni, M., Dabo, I., Dal Corso, A., de Gironcoli, S., Fabris, S., Fratesi, G., Gebauer, R., Gerstmann, U., Gougoussis, C., Kokalj, A., Lazzeri, M., Martin-Samos, L., Marzari, N., Mauri, F., Mazzarello, R., Paolini, S., Pasquarello, A., Paulatto, L., Sbraccia, C., Scandolo, S., Sclauzero, G., Seitsonen, A. P., Smogunov, A., Umari, P. & Wentzcovitch, R. M. (2009). *J. Phys. Condens. Matter*, **21**, 395502.

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

Hadjikakou, S. & Light, M. E. (2016). Private communication (refcode ODAXID). CCDC, Cambridge, England.

Haghverdi, M., Tadjarodi, A., Bahri–Laleh, N. & Nekoomanesh–Haghighi, M. (2018). *Appl. Organomet. Chem.* **32**, e4015.

Kenchappa, R., Bodke, Y. D., Telkar, S. & Aruna Sindhe, M. (2017). *J. Chem. Biol.* **10**, 11–23.

Kharitonova, M. I., Konstantinova, I. D. & Miroshnikov, A. I. (2018). *Russ. Chem. Rev.* **87**, 1111–1138.

Leila, Z., Zeinab, F., Kamiar, Z., Fatemeh Bi Bi, M., Asghar, J. & Soghra, K. (2019). *Res. Pharma. Sci.* **14**, 504–514.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Rathore, A., Sudhakar, R., Ahsan, M. J., Ali, A., Subbarao, N., Jadav, S. S., Umar, S. & Yar, M. S. (2017). *Bioorg. Chem.* **70**, 107–117.

Rigaku OD (2018). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.

Samanta, S., Lim, T. L. & Lam, Y. (2013). *ChemMedChem*, **8**, 994–1001.

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

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

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17.* University of Western Australia. http://Hirshfeldsurface.net

Xi, C., Sun, Z. & Liu, Y. (2013). *Dalton Trans.* **42**, 13327–13330.

supporting information

Acta Cryst. (2022). E**78**, 231-234 [https://doi.org/10.1107/S2056989022000792]

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

Dilnoza Rakhmonova, Lobar Gapurova, Surayyo Razzoqova, Shakhnoza Kadirova, Batirbay Torambetov, Zukhra Kadirova and Svitlana Shishkina

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-1*H*-benzimidazole-2(3*H*)-thione

Crystal data

$C_7H_7N_3S$
M_r = 165.22
Monoclinic, *C*2/*c*
a = 16.1179 (14) Å
b = 11.8796 (11) Å
c = 16.5649 (15) Å
β = 91.974 (8)°
V = 3169.9 (5) Å^3
Z = 16
F(000) = 1376
D_x = 1.385 Mg m^{-3}
Mo *Kα* 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 $I > 2\sigma(I)$
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
$R[F^2 > 2\sigma(F^2)]$ = 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
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 1.8442P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −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)

	x	*y*	*z*	U_{iso}*/U_{eq}
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	0.69335 (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)	0.0009 (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)	0.0383 (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, º)

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)
C3B—C2B—H2B	120.4 (17)	C1A—C2A—H2A	122.0 (16)
C2B—C3B—C4B	120.3 (2)	C2A—C3A—C4A	120.6 (2)
C2B—C3B—N3B	119.0 (2)	C2A—C3A—N3A	118.8 (2)
C4B—C3B—N3B	120.6 (2)	C4A—C3A—N3A	120.5 (2)
C5B—C4B—C3B	122.0 (3)	C5A—C4A—C3A	122.0 (3)
C5B—C4B—H4B	122.1 (18)	C5A—C4A—H4A	120.0 (17)
C3B—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	120.8 (2)	C5A—C6A—N2A	132.3 (2)
N2B—C6B—C1B	106.3 (2)	C1A—C6A—N2A	106.1 (2)
N2B—C7B—N1B	106.8 (2)	N1A—C7A—N2A	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)
N1B—C1B—C6B—C5B	−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)

C6B—N2B—C7B—N1B	−0.8 (3)	C1A—N1A—C7A—N2A	−1.8 (3)
C6B—N2B—C7B—S1B	179.5 (2)	C1A—N1A—C7A—S1A	177.73 (19)
C1B—N1B—C7B—N2B	1.5 (3)	C6A—N2A—C7A—N1A	1.6 (3)
C1B—N1B—C7B—S1B	−178.68 (19)	C6A—N2A—C7A—S1A	−177.99 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*NA*···N3*B*	0.80 (3)	2.06 (3)	2.856 (3)	176 (3)
N2*A*—H2*NA*···S1*B*^{i}	0.82 (3)	2.54 (3)	3.295 (2)	154 (3)
N3*A*—H3*NA*···S1*A*^{ii}	0.84 (4)	2.75 (4)	3.551 (3)	159 (3)
N3*A*—H3*NB*···C4*B*^{iii}	0.89 (4)	2.71 (4)	3.483 (4)	145 (3)
N3*A*—H3*NB*···C5*B*^{iii}	0.89 (4)	2.81 (4)	3.643 (4)	155 (3)
N1*B*—H1*NB*···N3*A*^{iv}	0.88 (3)	2.02 (3)	2.884 (3)	171 (3)
N2*B*—H2*NB*···S1*A*^{v}	0.85 (3)	2.56 (3)	3.340 (2)	153 (3)
N3*B*—H3*NC*···S1*B*^{vi}	0.86 (3)	2.91 (3)	3.672 (3)	149 (2)
N3*B*—H3*ND*···S1*B*^{vii}	0.85 (3)	2.70 (3)	3.477 (3)	153 (3)
C5*A*—H5*A*···S1*A*^{viii}	0.96 (3)	2.96 (3)	3.656 (3)	130.2 (19)
C5*B*—H5*B*···C1*A*^{ii}	0.90 (3)	2.78 (3)	3.562 (4)	147 (3)

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.