

Crystal structures of 2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine and 7-bromo-2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine

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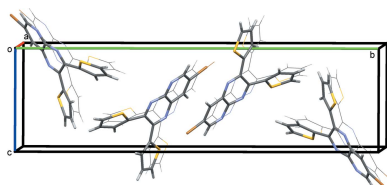
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The crystal structures of 2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine, C₁₅H₉N₃S₂ (**1**), and 7-bromo-2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine, C₁₅H₈BrN₃S₂ (**2**), are discussed. Both molecules crystallize in space group *P*2₁/*c*. In **1**, the thienyl rings are inclined to the mean plane of the pyridopyrazine moiety by 6.16 (7) and 86.66 (8)°, where as in **2** the corresponding dihedral angles are 33.29 (11) and 19.84 (9)°. The pyridopyrazine moiety is relatively planar in **1** with the two rings being inclined to each other by 1.33 (7)°. In **2**, however, the pyridopyrazine moiety is buckled with the corresponding dihedral angle being larger at 8.78 (10)°. In the crystal of **1**, the packing creates intersecting bilayers; the layering results from the pyridopyrazine moieties being engaged in offset π -stacking, where the interplanar distance is 3.431 (9) Å with an offset 1.14 Å. In the crystal of **2**, the molecules pack head-to-head and are linked by a series of C—H···Br and C—H···N intermolecular interactions, forming layers parallel to the *ab* plane.

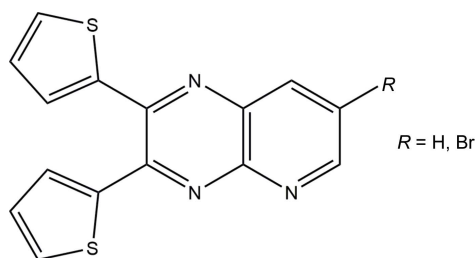
1. Chemical context

Nitrogen-containing heterocyclic aryl substituents at the 2- and 2,3- positions on quinoxalines have been shown repeatedly to engage in bidentate behavior in binding metals, utilizing the quinoxaline nitrogen atom. For example, 2-(2-pyridyl)quinoxaline has shown bidentate behavior with a variety of metals; focusing on silver, specifically, it can form 1:1 complexes assembling in one-dimensional chains (Shanmuga Sundara Raj *et al.*, 1999) or form 2:1 mononuclear complexes (Bi *et al.*, 2009) to cite just a few. With that bidentate behavior in mind, we aimed to test the bonding capabilities of thienyl sulfur atoms at the 2-, and 2,3- positions on mono- and dithienylquinoxalines. Thienyl-substituted quinoxalines have been shown to form bis-complexes with silver(I) (Crundwell *et al.*, 2014; Crundwell, 2013); however, so far we have not seen (N,S) bidentate behavior from the nitrogen on the quinoxaline and sulfur on the thienyl ring with a metal.

Monothienyl and/or 2,3-dithienyl-substituted pyrido[2,3-*b*]pyrazines are interesting ligands related to their quinoxaline analogs since they have an additional heterocyclic nitrogen atom. This could potentially create novel silver(I) frameworks and allow insight into the preference of silver when it binds to the heterocycles in these ligands. To date, little work has been done with monothienylpyrido[2,3-*b*]pyrazines or 2,3-dithienylpyrido[2,3-*b*]pyrazines. The crystal structure of 3-(2-thienyl)pyrido[2,3-*b*]pyrazine has been determined (Lassagne *et al.*, 2015). A few other 2,3-diarylpyrido[2,3-*b*]pyrazines and their subsequent metal complexes have been characterized through



diffraction studies. The crystal structure of 2,3-di(1*H*-2-pyrrolyl)pyrido[2,3-*b*]pyrazine, which is a colorimetric ion sensor, has been determined as well as a nickel(II) complex in which two ligands bind to the nickel via the outermost nitrogen atom on the pyridopyrazine moiety (Ghosh *et al.*, 2006). Rhenium(I) complexes with the generic formula [ReBr(CO)₃(*L*)] have been synthesized with a few 2,3-di-arylpyrido[2,3-*b*]pyrazines (Yeo *et al.*, 2010). These complexes are interesting because they utilize both nitrogen atoms on the same side of the pyridopyrazine moiety to bind the metal.



2. Structural details

The molecular structure of compound **1** is shown in Fig. 1. One of the two thienyl rings (C8–C11/S1) is nearly coplanar with the pyridopyrazine ring [the dihedral angle being 6.16 (7)°], therefore making most of the molecule appear flat. The r.m.s. deviation for all non-hydrogen atoms in the pyridopyrazine moiety and the nearly coplanar thiophene ring (C8–C11/S1) is only 0.0123 (16) Å. The mean plane of the other thienyl ring (C12–C15/S2) is nearly perpendicular to the plane created by the rest of the molecule, forming an angle of 86.67 (4)°. Finally, although unsubstituted thienyl ring-flip disorders are common on unsubstituted 2- or 3-thienyl rings (Crundwell *et al.*, 2003), there was not enough evidence of such a disorder to include it in the refinement model for **1**.

The molecular structure of compound **2** is shown in Fig. 2. This bromo derivative is less planar than the unbrominated compound **1**. The r.m.s. atomic displacement for the non-hydrogen atoms in the pyridopyrazine ring is 0.104 (2) Å. The

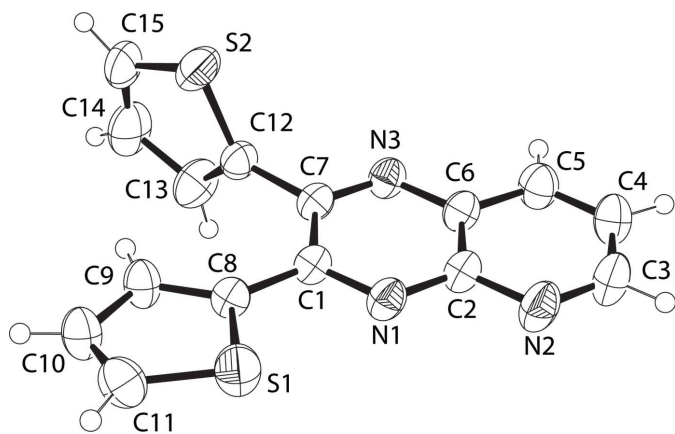


Figure 1

A view of the molecular structure of compound **1**, with the atom labeling and displacement ellipsoids drawn at the 50% probability level.

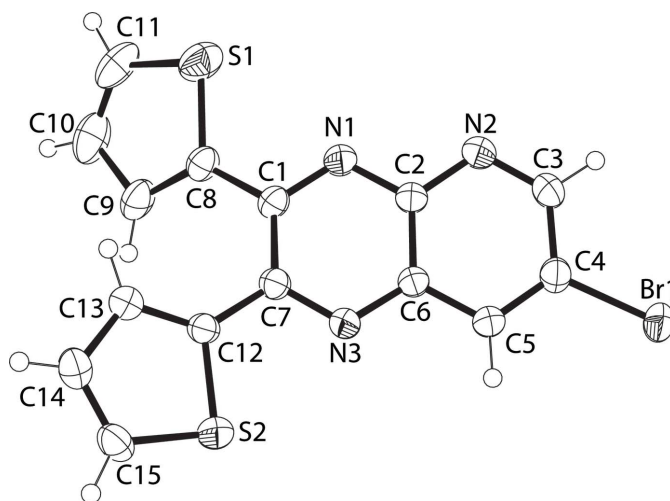


Figure 2

A view of the molecular structure of compound **2**, with the atom labeling and displacement ellipsoids drawn at the 50% probability level.

mean planes of the thienyl rings (C8–C11/S1 and C12–C15/S2) form angles of 33.29 (11) and 19.84 (9)°, respectively, with the mean plane of the pyridopyrazine moiety. The latter is buckled with the pyrazine and pyridine rings being inclined to each other by 8.78 (10)°, compared to only 1.33 (7)° in **1**.

All bond lengths and angles in both compounds **1** and **2** are within expected values and close to those reported for similar compounds (see *Database survey*).

3. Supramolecular Features

In the crystal of **1**, the packing can be described as a series of bilayers (Fig. 3). Using *Mercury* software (Macrae *et al.*, 2008) for the analysis, it can be seen that the molecules lie in planes with an offset π -stacking distance of 3.431 (9) Å, measured between the planar thienyl ring in one molecule and a portion of the pyridopyrazine ring system of a neighboring molecule.

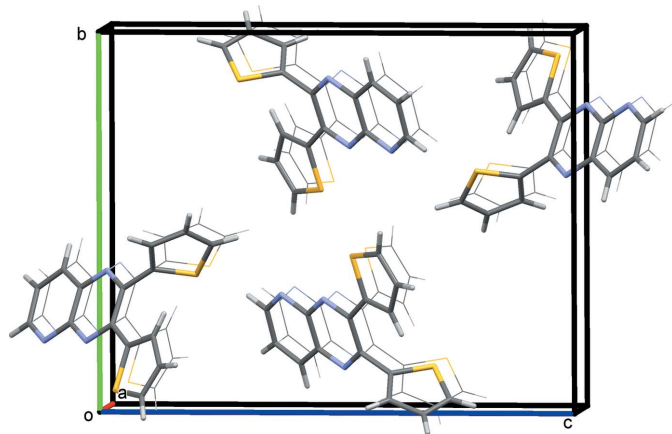


Figure 3

A view along the *a* axis of the crystal packing of compound **1**. Extra molecules were added to illustrate the stacking that occurs in planes.

Table 1
Hydrogen-bond geometry (Å, °) for **2**.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C3-H3\cdots Br1^i$	0.93	3.01	3.836 (1)	150
$C5-H5\cdots Br1^{ii}$	0.93	3.05	3.851 (1)	145
$C15-H15\cdots N1^{iii}$	0.93	2.65	3.572 (1)	175
$C11-H11\cdots C14^{iv}$	0.93	2.78	3.637 (1)	155

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

There are two other types of very weak intermolecular interactions in the crystal. The thienyl-ring sulfur atom S1 points directly at a neighboring inversion-related co-planar thienyl-ring sulfur atom at a distance of 3.570 (8) Å, roughly comparable to the sum of the van der Waals radii (3.8 Å). In addition, the pyridopyrazine hydrogen atom H3 is in a position to interact with the sp^2 carbon atom C15ⁱ on the tilted thienyl ring (C12–C15/S2) at (i) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$, at a distance of 2.870 (8) Å and forming an angle $C3-H3\cdots C15^i$ of 152.37 (8)°. These interactions are shown as colored dotted lines in Fig. 4.

In the crystal of the brominated derivative **2**, molecules pack through a number of intermolecular interactions (Fig. 5, Table 1). Several interactions between the bromine atoms and neighboring hydrogens create a head-to-head, sheet-like structure (Fig. 6). Bromine atoms form $C-H\cdots Br$ contacts at distances of 3.005 and 3.049 Å with the hydrogen atoms on C5 and C3, respectively. Within the same plane there are also interactions between the pyridopyrazine nitrogen atom, N1, and adjacent thienyl-ring hydrogen atoms on C15 at 2.645 Å. Finally, two types of interactions that connect molecules between planes are also present. A thienyl-ring hydrogen (on C11) is in contact with an sp^2 carbon (C14) in another layer at 2.775 Å and the π -system of the C12–C15/S2 thienyl ring is stacked over a neighboring pyridopyrazine moiety at 3.394 (9) Å. These interactions are shown as colored dotted lines in Fig. 6.

4. Database Survey

A search of the CSD (Version 5.39, August 2018 update; Groom *et al.*, 2016) revealed the crystal structures of two other

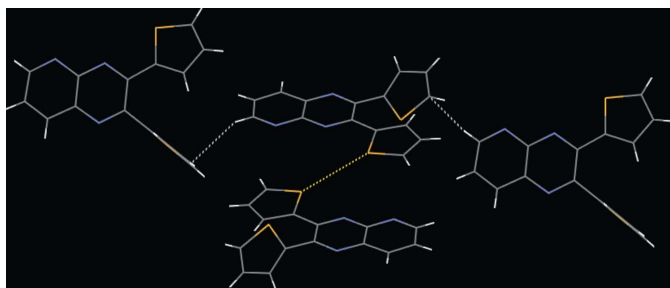


Figure 4
Intermolecular interactions in the crystal of **1**. The $S\cdots S$ interactions are shown as dotted yellow lines. The $C-H\cdots\pi$ (thienyl ring) interactions are shown in white.

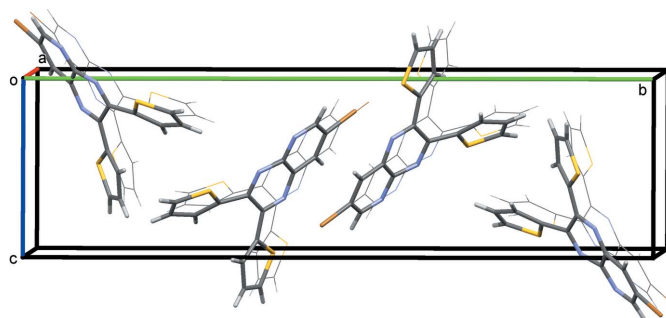


Figure 5
A view along the a axis of the crystal packing of compound **2**. Extra molecules were added to illustrate the stacking that occurs in planes.

arylpyrido[2,3-*b*]pyrazines, in addition to those already mentioned in the *Chemical context* section. In 7-bromo-3-[4-(piperidin-1-yl)phenyl]pyrido[2,3-*b*]pyrazine, the brominated pyridopyrazine ring remains coplanar with its aryl substituent (CSD refcode MUPVOK; Kekesi *et al.*, 2014). The same result is not found for 2,3-bis(5-bromo-1*H*-indol-3-yl)-7-chloropyrido[2,3-*b*]pyrazine acetone monosolvate (JUGCOF; Manivannan *et al.*, 2015), whose conformation resembles that of compound **2**, with both substituents being inclined to the mean plane of the pyridopyrazine ring.

Pyrido[2,3-*b*]pyrazines without halogenated pyridopyrazine rings are prevalent in the literature. Examples include: 2-(4-fluorophenyl)-3-(pyridin-4-yl)pyrido[2,3-*b*]pyrazine (BUDYAB; Koch *et al.*, 2009*a*), 4-[3-(4-fluorophenyl)pyrido[2,3-*b*]pyrazin-2-yl]-*N*-isopropylpyridin-2-amine (BUFBAG; Koch *et al.*, 2009*c*), 3-(4-fluorophenyl)-2-(pyridin-4-yl)pyrido[2,3-*b*]pyrazine (PUFNUA; Koch *et al.*, 2009*b*), 4,4'-pyrido[2,3-*b*]pyrazine-2,3-diylbis(*N,N*-diphenylaniline) (WUDQAO,

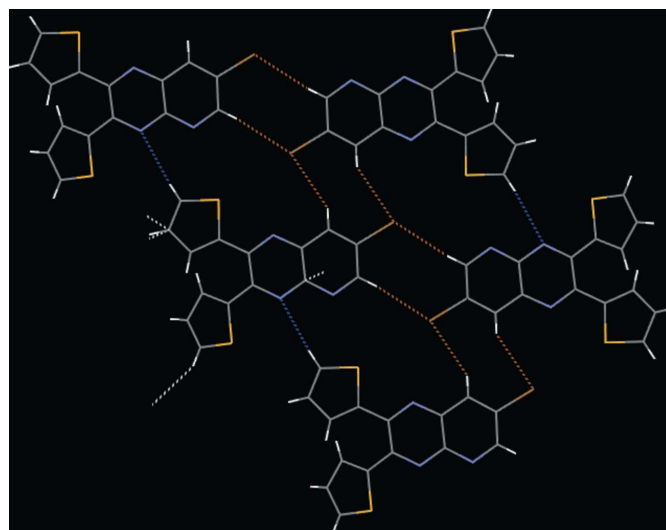


Figure 6
Intermolecular interactions in the crystal of **2**, highlighting the two-dimensional network of $C-H\cdots Br$ (brown dotted lines) and $C-H\cdots N$ (blue dotted lines) interactions that lie in the same plane. The dangling contacts on the thienyl rings, indicating $C-H\cdots\pi$ (thienyl ring) and $C-H\cdots\pi$ (pyridopyrazine) interactions, are shown with white dotted lines.

Table 2
Experimental details.

	1	2
Crystal data		
Chemical formula	C ₁₅ H ₉ N ₃ S ₂	C ₁₅ H ₈ BrN ₃ S ₂
<i>M_r</i>	295.37	374.27
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	293	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.25147 (12), 14.1093 (3), 17.7690 (3)	5.8336 (2), 29.4731 (10), 8.3160 (3)
β (°)	92.0296 (18)	95.466 (3)
<i>V</i> (Å ³)	1315.76 (4)	1423.30 (9)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.40	3.18
Crystal size (mm)	0.43 × 0.33 × 0.21	0.33 × 0.24 × 0.22
Data collection		
Diffractometer	Rigaku Xcalibur Sapphire3	Rigaku Xcalibur Sapphire3
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)
<i>T_{min}</i> , <i>T_{max}</i>	0.948, 1.000	0.455, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	19251, 4763, 3491	34519, 5255, 4166
<i>R_{int}</i>	0.021	0.034
(sin θ/λ) _{max} (Å ⁻¹)	0.773	0.785
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.148, 1.01	0.043, 0.110, 1.08
No. of reflections	4763	5255
No. of parameters	181	190
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.44, -0.40	0.63, -0.67

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

WUDQAO01; Xu *et al.*, 2015) and 4',4''-(pyrido[2,3-*b*]pyrazine-2,3-diyl)bis[(1,1'-biphenyl)-4-carbonitrile]chloroform monosolvate (YEMQUF; Gupta *et al.*, 2018). In all of these structures, both substituents are inclined to the mean plane of the pyridopyrazine ring, similar to the situation in compound **2**.

5. Synthesis and crystallization

All reagents were purchased from Sigma Aldrich and used without purification. Both molecules were synthesized by reacting equimolar amounts of the corresponding 2,3-diaminopyridines with 2,2'-thenil in refluxing glacial acetic acid.

2,3-Bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine (1): To a 250 ml round-bottom flask equipped with a magnetic stir bar were added 0.570 g of 2,3-diaminopyridine (5.23 mmol), 1.160 g of 2,2'-thenil (5.23 mmol), and 150 ml of glacial acetic acid. The solution was stirred, heated to boiling, and refluxed for 3 h. The resulting yellowish-brown solution was poured into a 250 ml beaker filled with ice, neutralized with sodium hydroxide, and isolated using vacuum filtration. A rough yield of the yellow-brown solid was 1.332 g (77%). The product was purified via column chromatography (SiO₂, 80% EtOAc/20% hexane, *R_f* = 0.75) to yield 1.010 g of compound **1** (m.p. 451 K). ATR-IR (cm⁻¹) 3101, 1541, 1453, 1409, 1359, 1257, 1092; ¹H NMR (300 MHz, CDCl₃): δ 9.50 (*d*, 1H), 8.79 (*d*, 1H), 7.90 (*dd*, 1H), 7.59 (*m*, 2H), 7.38 (*dd*, 2H), 7.10 (*m*, 2H); ¹³C NMR (300 MHz, CDCl₃): δ 154.28, 149.68, 149.31, 147.68, 141.17,

140.56, 137.63, 135.62, 130.60, 130.46, 129.96, 129.45, 127.70, 127.64, 125.12. Yellow plate-like crystals of **1** were obtained by slow evaporation of a solution in an equal volume mixture of toluene and ethanol.

7-Bromo-2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine (2): The above method was used for the brominated derivative by using 5-bromo-2,3-diaminopyridine as the starting diamine (m.p. 445 K); ATR-IR (cm⁻¹) 3099, 1539, 1427, 1410, 1331, 1311, 1237, 1172, 1072; ¹H NMR (300 MHz, CDCl₃): δ 9.10 (*d*, 1H), 8.58 (*d*, 1H), 7.59 (*m*, 2H), 7.46 (*m*, 2H), 7.10 (*m*, 2H); ¹³C NMR (300 MHz, CDCl₃): δ 155.14, 149.73, 148.44, 148.03, 140.83, 140.36, 138.89, 135.82, 130.88, 130.66, 130.33, 130.07, 127.78, 127.72, 120.81. Yellow plate-like crystals of **2** were obtained by slow evaporation of a solution in an equal volume mixture of toluene and ethanol. ¹H, FTIR, and COSY NMR spectra for **2** are given in the supporting information.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All the hydrogen atoms were constrained at ideal positions and refined using a riding model: C-H = 0.93 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C). In both compounds, some reflections were omitted because they were either partially obstructed by the beam stop or they had an Error/e.s.d. ratio higher than 5.00 where Error = Σ(*D*)(*wD*²/*wD*²)^{0.5}, *D* being *F_c*² - *F_o*².

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supporting information

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Crystal structures of 2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine and 7-bromo-2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine

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Computing details

For both structures, 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: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2,3-Bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine (1)

Crystal data

C₁₅H₉N₃S₂

M_r = 295.37

Monoclinic, *P*2₁/*c*

a = 5.25147 (12) Å

b = 14.1093 (3) Å

c = 17.7690 (3) Å

β = 92.0296 (18)°

V = 1315.76 (4) Å³

Z = 4

F(000) = 608

D_x = 1.491 Mg m⁻³

Melting point: 451 K

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 6256 reflections

θ = 4.5–32.1°

μ = 0.40 mm⁻¹

T = 293 K

Plate, yellow

0.43 × 0.33 × 0.21 mm

Data collection

Rigaku Xcalibur Sapphire3

diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: 16.1790 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Rigaku OD, 2018)

T_{min} = 0.948, *T_{max}* = 1.000

19251 measured reflections

4763 independent reflections

3491 reflections with *I* > 2σ(*I*)

R_{int} = 0.021

θ_{max} = 33.3°, θ_{min} = 4.1°

h = -8→6

k = -21→21

l = -27→26

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.048

wR(*F*²) = 0.148

S = 1.01

4763 reflections

181 parameters

0 restraints

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0773*P*)² + 0.306*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.44 e Å⁻³

Δρ_{min} = -0.40 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.29005 (9)	0.07264 (3)	0.05184 (3)	0.05601 (15)
S2	0.68406 (10)	0.36939 (5)	0.21271 (3)	0.0735 (2)
N3	0.8135 (2)	0.37660 (8)	0.02149 (7)	0.0390 (3)
N1	0.6466 (3)	0.19393 (8)	−0.01845 (7)	0.0407 (3)
C1	0.5489 (3)	0.23948 (9)	0.03890 (7)	0.0358 (3)
C7	0.6384 (3)	0.33311 (9)	0.05955 (7)	0.0356 (3)
C8	0.3498 (3)	0.18831 (9)	0.07804 (8)	0.0371 (3)
C12	0.5459 (3)	0.38619 (10)	0.12539 (8)	0.0401 (3)
C2	0.8310 (3)	0.23713 (10)	−0.05676 (8)	0.0387 (3)
C6	0.9139 (3)	0.32947 (10)	−0.03738 (8)	0.0381 (3)
N2	0.9315 (3)	0.18788 (10)	−0.11470 (8)	0.0531 (3)
C11	0.0556 (4)	0.06156 (12)	0.11368 (11)	0.0539 (4)
H11	−0.0380	0.0063	0.1198	0.065*
C9	0.1873 (3)	0.21596 (11)	0.13489 (9)	0.0439 (3)
H9	0.1894	0.2753	0.1576	0.053*
C10	0.0188 (3)	0.14123 (12)	0.15320 (10)	0.0523 (4)
H10	−0.1050	0.1470	0.1891	0.063*
C5	1.1070 (3)	0.37201 (11)	−0.07888 (10)	0.0483 (3)
H5	1.1647	0.4329	−0.0676	0.058*
C4	1.2062 (4)	0.32159 (14)	−0.13583 (10)	0.0532 (4)
H4	1.3348	0.3471	−0.1642	0.064*
C3	1.1122 (4)	0.23039 (14)	−0.15125 (10)	0.0567 (4)
H3	1.1835	0.1973	−0.1906	0.068*
C13	0.3588 (4)	0.45253 (13)	0.12665 (11)	0.0561 (4)
H13	0.2629	0.4718	0.0844	0.067*
C15	0.4890 (4)	0.45263 (18)	0.25111 (12)	0.0691 (6)
H15	0.4964	0.4701	0.3016	0.083*
C14	0.3271 (5)	0.48905 (15)	0.20032 (13)	0.0655 (5)
H14	0.2047	0.5340	0.2116	0.079*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0634 (3)	0.0423 (2)	0.0634 (3)	−0.00914 (17)	0.0164 (2)	−0.01125 (18)
S2	0.0567 (3)	0.1255 (5)	0.0382 (2)	0.0178 (3)	−0.00148 (19)	−0.0182 (3)
N3	0.0466 (6)	0.0332 (5)	0.0375 (6)	0.0006 (4)	0.0055 (5)	−0.0017 (4)

N1	0.0509 (6)	0.0359 (6)	0.0356 (6)	-0.0007 (5)	0.0059 (5)	-0.0035 (4)
C1	0.0410 (6)	0.0336 (6)	0.0327 (6)	0.0021 (5)	0.0022 (5)	0.0003 (5)
C7	0.0407 (6)	0.0335 (6)	0.0327 (6)	0.0022 (5)	0.0018 (5)	-0.0016 (5)
C8	0.0419 (6)	0.0331 (6)	0.0365 (6)	0.0003 (5)	0.0031 (5)	0.0011 (5)
C12	0.0448 (7)	0.0396 (7)	0.0363 (6)	-0.0041 (5)	0.0049 (5)	-0.0068 (5)
C2	0.0473 (7)	0.0361 (6)	0.0329 (6)	0.0031 (5)	0.0053 (5)	-0.0010 (5)
C6	0.0455 (7)	0.0352 (6)	0.0337 (6)	0.0023 (5)	0.0046 (5)	0.0013 (5)
N2	0.0690 (9)	0.0478 (7)	0.0437 (7)	-0.0010 (6)	0.0165 (6)	-0.0107 (6)
C11	0.0544 (9)	0.0437 (8)	0.0639 (11)	-0.0095 (7)	0.0064 (8)	0.0063 (7)
C9	0.0480 (7)	0.0358 (6)	0.0487 (8)	-0.0013 (6)	0.0157 (6)	0.0026 (6)
C10	0.0527 (9)	0.0508 (9)	0.0544 (9)	-0.0041 (7)	0.0159 (7)	0.0061 (7)
C5	0.0544 (9)	0.0436 (8)	0.0474 (8)	-0.0045 (6)	0.0103 (7)	0.0025 (6)
C4	0.0563 (9)	0.0572 (10)	0.0474 (8)	-0.0011 (7)	0.0173 (7)	0.0046 (7)
C3	0.0684 (11)	0.0590 (10)	0.0439 (8)	0.0037 (8)	0.0201 (8)	-0.0072 (7)
C13	0.0728 (11)	0.0462 (8)	0.0495 (9)	0.0139 (8)	0.0069 (8)	-0.0080 (7)
C15	0.0678 (11)	0.0904 (15)	0.0505 (10)	-0.0221 (11)	0.0229 (9)	-0.0331 (10)
C14	0.0807 (13)	0.0528 (10)	0.0645 (12)	0.0034 (9)	0.0221 (10)	-0.0199 (9)

Geometric parameters (Å, °)

S1—C8	1.7229 (14)	N2—C3	1.314 (2)
S1—C11	1.686 (2)	C11—H11	0.9300
S2—C12	1.7060 (15)	C11—C10	1.343 (3)
S2—C15	1.716 (2)	C9—H9	0.9300
N3—C7	1.3131 (18)	C9—C10	1.422 (2)
N3—C6	1.3613 (18)	C10—H10	0.9300
N1—C1	1.3236 (18)	C5—H5	0.9300
N1—C2	1.3486 (19)	C5—C4	1.356 (2)
C1—C7	1.4452 (19)	C4—H4	0.9300
C1—C8	1.466 (2)	C4—C3	1.402 (3)
C7—C12	1.4852 (19)	C3—H3	0.9300
C8—C9	1.401 (2)	C13—H13	0.9300
C12—C13	1.358 (2)	C13—C14	1.422 (3)
C2—C6	1.413 (2)	C15—H15	0.9300
C2—N2	1.3637 (19)	C15—C14	1.322 (4)
C6—C5	1.409 (2)	C14—H14	0.9300
C11—S1—C8	92.41 (8)	C10—C11—H11	123.7
C12—S2—C15	91.49 (10)	C8—C9—H9	124.5
C7—N3—C6	117.71 (12)	C8—C9—C10	111.02 (14)
C1—N1—C2	118.29 (12)	C10—C9—H9	124.5
N1—C1—C7	120.52 (12)	C11—C10—C9	113.49 (16)
N1—C1—C8	115.38 (12)	C11—C10—H10	123.3
C7—C1—C8	124.10 (12)	C9—C10—H10	123.3
N3—C7—C1	121.59 (12)	C6—C5—H5	121.0
N3—C7—C12	115.14 (12)	C4—C5—C6	118.02 (15)
C1—C7—C12	123.26 (12)	C4—C5—H5	121.0
C1—C8—S1	117.68 (10)	C5—C4—H4	120.5

C9—C8—S1	110.41 (11)	C5—C4—C3	119.03 (15)
C9—C8—C1	131.91 (13)	C3—C4—H4	120.5
C7—C12—S2	120.39 (11)	N2—C3—C4	125.32 (15)
C13—C12—S2	111.44 (12)	N2—C3—H3	117.3
C13—C12—C7	128.15 (15)	C4—C3—H3	117.3
N1—C2—C6	120.97 (12)	C12—C13—H13	124.0
N1—C2—N2	117.05 (13)	C12—C13—C14	111.93 (18)
N2—C2—C6	121.98 (14)	C14—C13—H13	124.0
N3—C6—C2	120.89 (13)	S2—C15—H15	124.0
N3—C6—C5	119.97 (13)	C14—C15—S2	111.93 (15)
C5—C6—C2	119.13 (13)	C14—C15—H15	124.0
C3—N2—C2	116.51 (14)	C13—C14—H14	123.4
S1—C11—H11	123.7	C15—C14—C13	113.20 (18)
C10—C11—S1	112.65 (13)	C15—C14—H14	123.4
S1—C8—C9—C10	-0.99 (18)	C7—C12—C13—C14	-178.93 (16)
S1—C11—C10—C9	-0.9 (2)	C8—S1—C11—C10	0.26 (16)
S2—C12—C13—C14	-0.7 (2)	C8—C1—C7—N3	-178.50 (13)
S2—C15—C14—C13	-1.6 (3)	C8—C1—C7—C12	2.9 (2)
N3—C7—C12—S2	-92.59 (15)	C8—C9—C10—C11	1.2 (2)
N3—C7—C12—C13	85.5 (2)	C12—S2—C15—C14	1.07 (18)
N3—C6—C5—C4	178.33 (15)	C12—C13—C14—C15	1.5 (3)
N1—C1—C7—N3	1.6 (2)	C2—N1—C1—C7	0.0 (2)
N1—C1—C7—C12	-176.99 (13)	C2—N1—C1—C8	-179.89 (12)
N1—C1—C8—S1	6.41 (17)	C2—C6—C5—C4	-0.4 (2)
N1—C1—C8—C9	-172.69 (15)	C2—N2—C3—C4	-0.6 (3)
N1—C2—C6—N3	1.3 (2)	C6—N3—C7—C1	-1.7 (2)
N1—C2—C6—C5	-179.99 (14)	C6—N3—C7—C12	177.03 (12)
N1—C2—N2—C3	-179.52 (16)	C6—C2—N2—C3	0.7 (2)
C1—N1—C2—C6	-1.4 (2)	C6—C5—C4—C3	0.5 (3)
C1—N1—C2—N2	178.84 (14)	N2—C2—C6—N3	-178.93 (14)
C1—C7—C12—S2	86.08 (16)	N2—C2—C6—C5	-0.3 (2)
C1—C7—C12—C13	-95.8 (2)	C11—S1—C8—C1	-178.84 (12)
C1—C8—C9—C10	178.15 (15)	C11—S1—C8—C9	0.44 (13)
C7—N3—C6—C2	0.3 (2)	C5—C4—C3—N2	0.0 (3)
C7—N3—C6—C5	-178.40 (13)	C15—S2—C12—C7	178.22 (13)
C7—C1—C8—S1	-173.50 (11)	C15—S2—C12—C13	-0.19 (15)
C7—C1—C8—C9	7.4 (2)		

7-Bromo-2,3-bis(thiophen-2-yl)pyrido[2,3-*b*]pyrazine (2)*Crystal data*C₁₅H₈BrN₃S₂*M_r* = 374.27Monoclinic, *P*2₁/*c**a* = 5.8336 (2) Å*b* = 29.4731 (10) Å*c* = 8.3160 (3) Å β = 95.466 (3)°*V* = 1423.30 (9) Å³*Z* = 4*F*(000) = 744*D_x* = 1.747 Mg m⁻³

Melting point: 445 K

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 9441 reflections

$\theta = 4.5\text{--}32.2^\circ$
 $\mu = 3.18 \text{ mm}^{-1}$
 $T = 293 \text{ K}$

Plate, yellow
 $0.33 \times 0.24 \times 0.22 \text{ mm}$

Data collection

Rigaku Xcalibur Sapphire3
 diffractometer
 Radiation source: Enhance (Mo) X-ray Source
 Graphite monochromator
 Detector resolution: 16.1790 pixels mm^{-1}
 ω scans
 Absorption correction: multi-scan
 (CrysAlis PRO; Rigaku OD, 2018)
 $T_{\min} = 0.455$, $T_{\max} = 1.000$

34519 measured reflections
 5255 independent reflections
 4166 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\max} = 33.9^\circ$, $\theta_{\min} = 4.2^\circ$
 $h = -8 \rightarrow 8$
 $k = -45 \rightarrow 45$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.08$
 5255 reflections
 190 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
 $w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.940P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.63 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.67 \text{ e } \text{Å}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.69446 (4)	0.018840 (9)	0.30276 (3)	0.04319 (9)
S2	0.62946 (10)	-0.11087 (2)	-0.49251 (7)	0.04132 (14)
S1	1.54351 (12)	-0.19256 (2)	-0.09942 (10)	0.05248 (18)
N3	0.8311 (3)	-0.08963 (6)	-0.1758 (2)	0.0312 (3)
C12	0.8921 (3)	-0.13124 (7)	-0.4089 (3)	0.0294 (4)
C7	0.9600 (3)	-0.12031 (7)	-0.2402 (2)	0.0290 (4)
C2	1.1218 (4)	-0.08478 (7)	0.0484 (3)	0.0314 (4)
C6	0.9043 (3)	-0.07298 (7)	-0.0283 (2)	0.0290 (4)
C13	1.0082 (4)	-0.15121 (8)	-0.5255 (3)	0.0354 (4)
H13	1.1549	-0.1635	-0.5056	0.042*
N1	1.2404 (3)	-0.11997 (7)	-0.0083 (2)	0.0342 (4)
N2	1.2152 (4)	-0.06423 (8)	0.1847 (3)	0.0428 (5)
C1	1.1566 (4)	-0.13963 (7)	-0.1436 (3)	0.0298 (4)

C5	0.7682 (4)	-0.04198 (8)	0.0495 (3)	0.0327 (4)
H5	0.6198	-0.0346	0.0066	0.039*
C4	0.8620 (4)	-0.02319 (7)	0.1898 (3)	0.0330 (4)
C8	1.2653 (4)	-0.18271 (7)	-0.1791 (3)	0.0331 (4)
C14	0.8825 (4)	-0.15116 (8)	-0.6789 (3)	0.0386 (5)
H14	0.9366	-0.1637	-0.7707	0.046*
C15	0.6754 (4)	-0.13092 (8)	-0.6780 (3)	0.0395 (5)
H15	0.5699	-0.1283	-0.7686	0.047*
C3	1.0885 (4)	-0.03388 (9)	0.2503 (3)	0.0413 (5)
H3	1.1521	-0.0186	0.3419	0.050*
C9	1.1615 (5)	-0.22302 (8)	-0.2534 (3)	0.0445 (6)
H9	1.0113	-0.2255	-0.3013	0.053*
C10	1.3303 (6)	-0.25845 (9)	-0.2402 (4)	0.0575 (8)
H10	1.3004	-0.2874	-0.2817	0.069*
C11	1.5344 (6)	-0.24684 (10)	-0.1638 (4)	0.0589 (8)
H11	1.6584	-0.2667	-0.1479	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04705 (15)	0.04449 (14)	0.03805 (13)	0.00908 (10)	0.00417 (10)	-0.01197 (10)
S2	0.0361 (3)	0.0475 (3)	0.0388 (3)	0.0120 (2)	-0.0047 (2)	-0.0046 (2)
S1	0.0458 (3)	0.0422 (3)	0.0694 (5)	0.0123 (3)	0.0051 (3)	0.0048 (3)
N3	0.0301 (8)	0.0319 (9)	0.0308 (8)	0.0037 (7)	-0.0023 (6)	-0.0041 (7)
C12	0.0274 (9)	0.0279 (9)	0.0320 (9)	0.0004 (7)	-0.0016 (7)	-0.0012 (7)
C7	0.0294 (9)	0.0272 (9)	0.0301 (9)	0.0005 (7)	0.0007 (7)	-0.0005 (7)
C2	0.0304 (9)	0.0329 (10)	0.0299 (9)	0.0045 (8)	-0.0019 (7)	-0.0015 (8)
C6	0.0291 (9)	0.0282 (9)	0.0291 (9)	0.0034 (7)	-0.0003 (7)	-0.0006 (7)
C13	0.0326 (10)	0.0393 (11)	0.0337 (10)	0.0016 (9)	0.0010 (8)	-0.0031 (9)
N1	0.0333 (9)	0.0353 (9)	0.0327 (9)	0.0084 (7)	-0.0031 (7)	-0.0012 (7)
N2	0.0382 (10)	0.0502 (12)	0.0376 (10)	0.0112 (9)	-0.0093 (8)	-0.0104 (9)
C1	0.0306 (9)	0.0267 (9)	0.0323 (10)	0.0038 (7)	0.0037 (7)	0.0003 (7)
C5	0.0306 (9)	0.0343 (10)	0.0323 (10)	0.0057 (8)	-0.0012 (8)	-0.0021 (8)
C4	0.0370 (10)	0.0316 (10)	0.0306 (10)	0.0021 (8)	0.0041 (8)	-0.0027 (8)
C8	0.0367 (10)	0.0285 (9)	0.0345 (10)	0.0057 (8)	0.0058 (8)	0.0030 (8)
C14	0.0479 (13)	0.0365 (11)	0.0313 (10)	-0.0003 (9)	0.0031 (9)	-0.0030 (8)
C15	0.0481 (13)	0.0368 (11)	0.0314 (11)	0.0015 (10)	-0.0085 (9)	-0.0011 (8)
C3	0.0432 (12)	0.0451 (13)	0.0334 (11)	0.0070 (10)	-0.0076 (9)	-0.0106 (9)
C9	0.0523 (14)	0.0343 (12)	0.0476 (13)	0.0153 (10)	0.0085 (11)	0.0000 (10)
C10	0.075 (2)	0.0290 (12)	0.072 (2)	0.0045 (12)	0.0257 (16)	-0.0035 (12)
C11	0.0594 (18)	0.0402 (14)	0.080 (2)	0.0221 (13)	0.0240 (16)	0.0075 (14)

Geometric parameters (Å, °)

Br1—C4	1.884 (2)	N1—C1	1.318 (3)
S2—C12	1.729 (2)	N2—C3	1.312 (3)
S2—C15	1.697 (2)	C1—C8	1.462 (3)
S1—C8	1.718 (2)	C5—H5	0.9300

S1—C11	1.686 (3)	C5—C4	1.358 (3)
N3—C7	1.321 (3)	C4—C3	1.404 (3)
N3—C6	1.352 (3)	C8—C9	1.446 (4)
C12—C7	1.457 (3)	C14—H14	0.9300
C12—C13	1.368 (3)	C14—C15	1.348 (3)
C7—C1	1.452 (3)	C15—H15	0.9300
C2—C6	1.408 (3)	C3—H3	0.9300
C2—N1	1.356 (3)	C9—H9	0.9300
C2—N2	1.353 (3)	C9—C10	1.432 (4)
C6—C5	1.408 (3)	C10—H10	0.9300
C13—H13	0.9300	C10—C11	1.339 (5)
C13—C14	1.410 (3)	C11—H11	0.9300
C15—S2—C12	91.95 (11)	C4—C5—H5	121.3
C11—S1—C8	92.17 (14)	C5—C4—Br1	120.71 (17)
C7—N3—C6	118.26 (18)	C5—C4—C3	120.3 (2)
C7—C12—S2	117.37 (15)	C3—C4—Br1	118.93 (17)
C13—C12—S2	110.13 (16)	C1—C8—S1	118.76 (17)
C13—C12—C7	132.08 (19)	C9—C8—S1	111.58 (17)
N3—C7—C12	115.37 (18)	C9—C8—C1	128.9 (2)
N3—C7—C1	119.60 (18)	C13—C14—H14	123.7
C1—C7—C12	125.02 (18)	C15—C14—C13	112.6 (2)
N1—C2—C6	119.96 (19)	C15—C14—H14	123.7
N2—C2—C6	122.8 (2)	S2—C15—H15	123.9
N2—C2—N1	117.08 (19)	C14—C15—S2	112.24 (17)
N3—C6—C2	120.93 (19)	C14—C15—H15	123.9
N3—C6—C5	120.64 (18)	N2—C3—C4	123.5 (2)
C5—C6—C2	118.38 (19)	N2—C3—H3	118.3
C12—C13—H13	123.5	C4—C3—H3	118.3
C12—C13—C14	113.0 (2)	C8—C9—H9	126.0
C14—C13—H13	123.5	C10—C9—C8	108.0 (3)
C1—N1—C2	118.22 (18)	C10—C9—H9	126.0
C3—N2—C2	117.1 (2)	C9—C10—H10	122.5
C7—C1—C8	124.32 (19)	C11—C10—C9	115.1 (3)
N1—C1—C7	120.60 (18)	C11—C10—H10	122.5
N1—C1—C8	114.94 (19)	S1—C11—H11	123.4
C6—C5—H5	121.3	C10—C11—S1	113.1 (2)
C4—C5—C6	117.4 (2)	C10—C11—H11	123.4
Br1—C4—C3—N2	176.7 (2)	C6—C2—N2—C3	3.8 (4)
S2—C12—C7—N3	-10.8 (3)	C6—C5—C4—Br1	179.77 (16)
S2—C12—C7—C1	170.70 (17)	C6—C5—C4—C3	1.6 (3)
S2—C12—C13—C14	-1.8 (3)	C13—C12—C7—N3	161.0 (2)
S1—C8—C9—C10	-1.7 (3)	C13—C12—C7—C1	-17.6 (4)
N3—C7—C1—N1	-16.0 (3)	C13—C14—C15—S2	0.8 (3)
N3—C7—C1—C8	159.4 (2)	N1—C2—C6—N3	-13.7 (3)
N3—C6—C5—C4	-173.5 (2)	N1—C2—C6—C5	168.7 (2)
C12—S2—C15—C14	-1.6 (2)	N1—C2—N2—C3	-172.1 (2)

C12—C7—C1—N1	162.4 (2)	N1—C1—C8—S1	-25.5 (3)
C12—C7—C1—C8	-22.2 (3)	N1—C1—C8—C9	143.6 (2)
C12—C13—C14—C15	0.7 (3)	N2—C2—C6—N3	170.5 (2)
C7—N3—C6—C2	5.8 (3)	N2—C2—C6—C5	-7.0 (4)
C7—N3—C6—C5	-176.7 (2)	N2—C2—N1—C1	-177.9 (2)
C7—C12—C13—C14	-174.0 (2)	C1—C8—C9—C10	-171.4 (2)
C7—C1—C8—S1	158.88 (17)	C5—C4—C3—N2	-5.1 (4)
C7—C1—C8—C9	-32.0 (4)	C8—S1—C11—C10	-1.2 (3)
C2—C6—C5—C4	4.0 (3)	C8—C9—C10—C11	0.9 (4)
C2—N1—C1—C7	8.1 (3)	C15—S2—C12—C7	175.40 (18)
C2—N1—C1—C8	-167.7 (2)	C15—S2—C12—C13	1.91 (19)
C2—N2—C3—C4	2.3 (4)	C9—C10—C11—S1	0.3 (4)
C6—N3—C7—C12	-170.23 (19)	C11—S1—C8—C1	172.6 (2)
C6—N3—C7—C1	8.4 (3)	C11—S1—C8—C9	1.7 (2)
C6—C2—N1—C1	6.1 (3)		

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C3—H3...Br1 ⁱ	0.93	3.01	3.836 (1)	150
C5—H5...Br1 ⁱⁱ	0.93	3.05	3.851 (1)	145
C15—H15...N1 ⁱⁱⁱ	0.93	2.65	3.572 (1)	175
C11—H11...C14 ^{iv}	0.93	2.78	3.637 (1)	155

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