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7-Bromo-2,3-bis[(prop-2-yn-1-yl)sulfanyl]pyrido-[2,3-*b*]pyrazine

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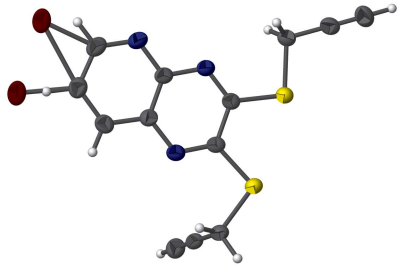
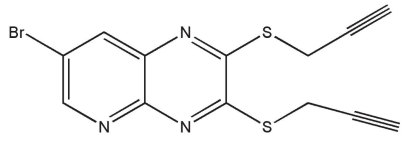
In the title compound, $C_{13}H_8BrN_3S_2$, one propynyl substituent lies approximately in the plane of the pyridopyrazine ring system, while the other is twisted away from this plane. In the crystal, offset π–π stacking interactions between the pyridine and pyrazine rings with a centroid–centroid distance of 3.740 (1) Å stack the molecules along the *a*-axis direction. At the conclusion of the initial refinement, a significant residual peak remained in the difference map. This suggested an alternate location for the Br atom but at a very low occupancy. Further refinement with Br disordered over two sites yielded a population ratio for the two Br sites of 97:3. As the refined location of the minor Br site leads to unequal C—C—Br angles, we feel that the results indicate a 'whole molecule' disorder rather than the presence of a minor amount of an isomer. Unfortunately, the very low amount of the second component of the disorder prevented the location of any of its other atoms.

3D view



Chemical scheme



Structure description

Pyrido-pyrazine heterocyclic compounds are important in organic chemistry and are also known to be important biologically (Richter *et al.*, 2006). Their uses include as anti-malarial agents (Shekhar *et al.*, 2014), anti-cancer drugs (Gong *et al.*, 2011), as anti-inflammatories (Hodgetts *et al.*, 2010) and as HIV-1 integrase inhibitors (Wai *et al.*, 2007). They are also used as inhibitors of anaplastic lymphoma kinase (Milkiewicz *et al.*, 2010). As a continuation of our research in the field of substituted pyrido[2,3-*b*]pyrazine derivatives (Hjouji *et al.*, 2014), we report here the synthesis of a new product by the

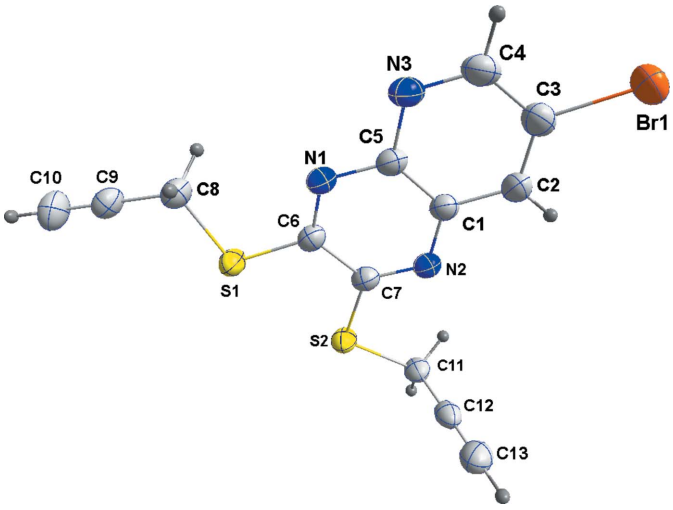


Figure 1
The title molecule with the labeling scheme and 50% probability displacement ellipsoids. Only the major disorder component is shown.

reaction of propargyl bromide with an excess of pyrido[2,3-*b*]pyrazine(1*H*,4*H*)-2,3-dithiol in dimethyl formamide in the presence of potassium carbonate and a catalytic quantity of tetra-*n*-butylammonium bromide. The structure of another pyrido [2,3-*b*]pyrazine derivative has been reported previously (Fun *et al.*, 2011).

In the title compound (Fig. 1), one propynyl substituent lies approximately in the plane of the pyridopyrazine ring system while the other is twisted away from this plane as shown by the C6—S1—C8—C9 [175.29 (17)°] and C7—S2—C11—C12 [76.78 (19)°] torsion angles. In the crystal, the molecules form stacks along the *a*-axis direction (Fig. 2) through offset π–π-stacking interactions between the pyridine and pyrazine rings (Fig. 3) with a centroid–centroid distance of 3.740 (1) Å and an interplanar separation of 3.440 (1) Å.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_8BrN_3S_2$
M_r	350.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	4.2159 (1), 16.7730 (5), 19.4656 (5)
β (°)	91.149 (1)
V (Å^3)	1376.20 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	6.81
Crystal size (mm)	0.20 × 0.08 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.46, 0.77
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21387, 2726, 2513
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.086, 1.05
No. of reflections	2726
No. of parameters	176
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.57

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

Propargyl bromide (0.16 ml, 1.82 mmol) was added to a solution of 7-bromopyrido[2,3-*b*]pyrazine-2,3-dithiol (0.2 g, 0.73 mmol), K_2CO_3 (0.3 g, 2.19 mmol), tetra-*n*-butyl ammonium bromide (0.03 g, 0.1 mmol) in DMF (10 ml). The mixture was then stirred for 6 h at room temperature. The solvent was

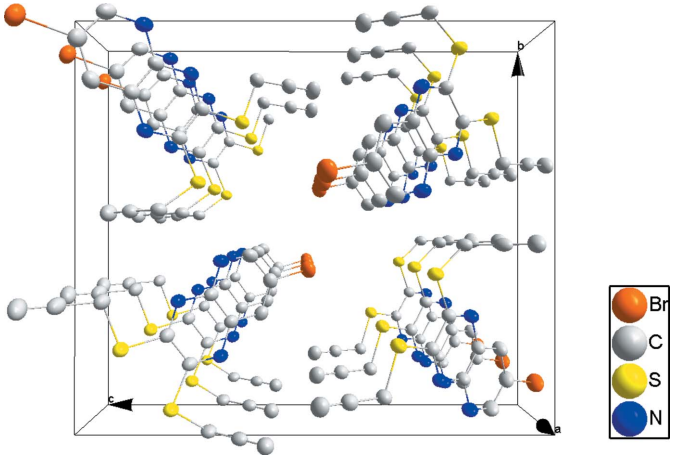


Figure 2
Packing of the title compound projected onto (100).

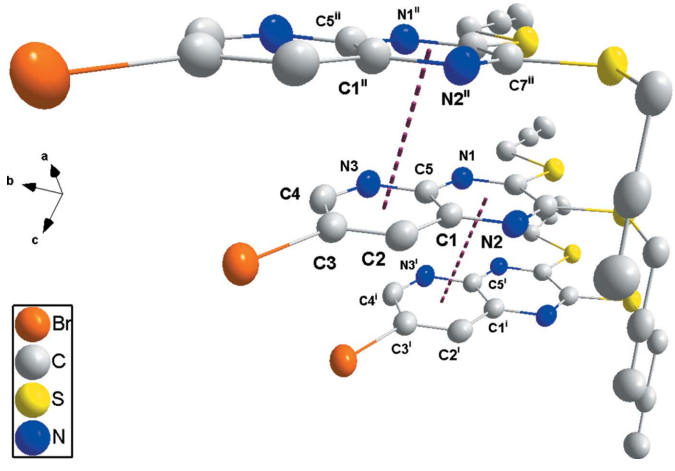


Figure 3
Details of the offset-π–π stacking. [Symmetry codes: (i) −1 + *x*, *y*, *z*; (ii) 1 + *x*, *y*, *z*.]

evaporated under reduced pressure and the product isolated by chromatography on a silica gel column with ethyl acetate/hexane (1/3) as eluent. The compound forms pale yellow columnar crystals in 20% yield and was recrystallized from a solvent mixture (dichloromethane–hexane: 1/2).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. At the conclusion of the initial refinement, a significant residual peak remained in the difference map at *ca* 1.85 Å from C4. This suggested an alternate location for Br1 but at a very low occupancy. Further refinement with Br1 disordered over two sites yielded a population ratio for the two Br sites of 97:3. As the refined location of the minor Br site leads to unequal C—C—Br angles, we feel that the results indicate a 'whole molecule' disorder rather than the presence of a minor amount of an isomer. Unfortunately, the very low amount of the second component of the disorder prevented the location of any of its other atoms.

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full crystallographic data

IUCrData (2016). **1**, x161881 [https://doi.org/10.1107/S2414314616018812]

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Crystal data

$C_{13}H_8BrN_3S_2$
M_r = 350.25
Monoclinic, $P2_1/c$
a = 4.2159 (1) Å
b = 16.7730 (5) Å
c = 19.4656 (5) Å
β = 91.149 (1)°
V = 1376.20 (6) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.690 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9904 reflections
θ = 3.5–72.4°
μ = 6.81 mm^{-1}
T = 150 K
Column, pale yellow
0.20 × 0.08 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.46, T_{max} = 0.77
21387 measured reflections
2726 independent reflections
2513 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 72.4°, θ_{min} = 3.5°
h = −5→5
k = −20→20
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.086
S = 1.05
2726 reflections
176 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.2838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms. At the conclusion of the initial refinement, a significant residual peak remained the difference map at ca. 1.85 Å from C4. This suggested an alternate location for Br1 but at a very low occupancy. Further refinement with Br1 disordered over two sites yielded a population ratio for the two Br sites of 97:3. Because the refined location of the minor Br site leads to unequal C–C–Br angles, we feel that the results indicate a "whole molecule" disorder rather than the presence of a minor amount of an isomer. Unfortunately, the very low amount of the second component of the disorder prevented location of any of its other atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	1.33510 (8)	0.89445 (2)	0.98676 (2)	0.05325 (13)	0.9711 (8)
C3	1.0987 (6)	0.87110 (17)	0.90621 (13)	0.0414 (6)	0.9711 (8)
C4	0.9795 (7)	0.93338 (16)	0.86557 (14)	0.0438 (6)	0.9711 (8)
H4	1.0330	0.9864	0.8784	0.053*	0.9711 (8)
Br1A	1.186 (3)	1.0075 (6)	0.9223 (5)	0.05325 (13)	0.0289 (8)
C3A	1.0987 (6)	0.87110 (17)	0.90621 (13)	0.0414 (6)	0.0289 (8)
H3A	1.2202	0.8812	0.9483	0.050*	0.0289 (8)
C4A	0.9795 (7)	0.93338 (16)	0.86557 (14)	0.0438 (6)	0.0289 (8)
S1	0.21077 (15)	0.74574 (3)	0.64709 (3)	0.03557 (15)	
S2	0.46504 (15)	0.60113 (3)	0.72597 (3)	0.03503 (15)	
N1	0.5283 (5)	0.83752 (11)	0.73672 (10)	0.0324 (4)	
N2	0.7585 (5)	0.70372 (12)	0.81113 (10)	0.0337 (4)	
N3	0.7976 (6)	0.92284 (12)	0.81063 (11)	0.0400 (5)	
C1	0.8373 (6)	0.78020 (14)	0.83001 (12)	0.0330 (5)	
C2	1.0335 (6)	0.79318 (16)	0.88808 (13)	0.0385 (5)	
H2	1.1184	0.7499	0.9140	0.046*	
C5	0.7232 (6)	0.84662 (14)	0.79321 (12)	0.0331 (5)	
C6	0.4557 (6)	0.76449 (14)	0.71894 (12)	0.0313 (5)	
C7	0.5753 (5)	0.69566 (13)	0.75688 (12)	0.0313 (5)	
C8	0.1351 (6)	0.84778 (14)	0.61874 (12)	0.0355 (5)	
H8A	0.0153	0.8770	0.6540	0.043*	
H8B	0.3383	0.8759	0.6117	0.043*	
C9	−0.0480 (6)	0.84493 (15)	0.55455 (13)	0.0378 (5)	
C10	−0.1994 (7)	0.84327 (18)	0.50324 (14)	0.0484 (7)	
H10	−0.3217	0.8419	0.4617	0.058*	
C11	0.6516 (6)	0.53851 (14)	0.79116 (12)	0.0343 (5)	
H11A	0.6691	0.4835	0.7731	0.041*	
H11B	0.8691	0.5583	0.8008	0.041*	
C12	0.4780 (6)	0.53656 (14)	0.85501 (13)	0.0355 (5)	
C13	0.3346 (7)	0.53361 (17)	0.90614 (15)	0.0467 (6)	
H13	0.2188	0.5312	0.9475	0.056*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0562 (2)	0.0577 (2)	0.04545 (19)	−0.01377 (14)	−0.01003 (14)	−0.00496 (13)
C3	0.0422 (14)	0.0438 (14)	0.0383 (13)	−0.0088 (11)	0.0013 (11)	−0.0023 (11)
C4	0.0508 (15)	0.0350 (13)	0.0456 (15)	−0.0115 (11)	0.0034 (12)	−0.0030 (11)
Br1A	0.0562 (2)	0.0577 (2)	0.04545 (19)	−0.01377 (14)	−0.01003 (14)	−0.00496 (13)
C3A	0.0422 (14)	0.0438 (14)	0.0383 (13)	−0.0088 (11)	0.0013 (11)	−0.0023 (11)
C4A	0.0508 (15)	0.0350 (13)	0.0456 (15)	−0.0115 (11)	0.0034 (12)	−0.0030 (11)
S1	0.0424 (3)	0.0295 (3)	0.0345 (3)	0.0006 (2)	−0.0039 (2)	0.0022 (2)
S2	0.0422 (3)	0.0260 (3)	0.0367 (3)	−0.0005 (2)	−0.0040 (2)	0.0007 (2)
N1	0.0370 (10)	0.0273 (9)	0.0330 (10)	0.0003 (8)	0.0024 (8)	0.0015 (8)
N2	0.0363 (10)	0.0287 (9)	0.0360 (10)	−0.0014 (8)	0.0004 (8)	0.0038 (8)
N3	0.0496 (12)	0.0284 (10)	0.0420 (12)	−0.0048 (9)	0.0006 (9)	0.0001 (9)
C1	0.0354 (12)	0.0307 (11)	0.0328 (11)	−0.0044 (9)	0.0026 (9)	0.0020 (9)
C2	0.0388 (13)	0.0399 (13)	0.0366 (13)	−0.0049 (10)	−0.0018 (10)	0.0063 (10)
C5	0.0381 (12)	0.0281 (11)	0.0333 (11)	−0.0024 (9)	0.0040 (9)	0.0022 (9)
C6	0.0330 (11)	0.0302 (11)	0.0310 (11)	0.0008 (9)	0.0037 (9)	0.0024 (9)
C7	0.0321 (11)	0.0279 (11)	0.0342 (11)	0.0007 (9)	0.0040 (9)	0.0026 (9)
C8	0.0418 (13)	0.0316 (12)	0.0332 (12)	0.0028 (10)	0.0010 (10)	0.0029 (9)
C9	0.0415 (13)	0.0353 (12)	0.0367 (13)	0.0063 (10)	0.0043 (10)	0.0035 (10)
C10	0.0532 (16)	0.0515 (16)	0.0401 (14)	0.0140 (13)	−0.0056 (12)	−0.0024 (12)
C11	0.0376 (12)	0.0255 (10)	0.0397 (12)	0.0013 (9)	−0.0025 (10)	0.0013 (9)
C12	0.0365 (12)	0.0272 (11)	0.0424 (13)	−0.0034 (9)	−0.0080 (10)	0.0009 (10)
C13	0.0525 (16)	0.0452 (15)	0.0423 (15)	−0.0083 (12)	0.0004 (12)	−0.0001 (12)

Geometric parameters (Å, º)

Br1—C3	1.882 (3)	N2—C1	1.373 (3)
C3—C2	1.380 (4)	N3—C5	1.358 (3)
C3—C4	1.398 (4)	C1—C2	1.404 (3)
C4—N3	1.315 (4)	C1—C5	1.404 (3)
C4—H4	0.9500	C2—H2	0.9500
Br1A—C4A	1.866 (4)	C6—C7	1.455 (3)
C3A—C2	1.380 (4)	C8—C9	1.456 (3)
C3A—C4A	1.398 (4)	C8—H8A	0.9900
C3A—H3A	0.9729	C8—H8B	0.9900
C4A—N3	1.315 (4)	C9—C10	1.175 (4)
S1—C6	1.750 (2)	C10—H10	0.9500
S1—C8	1.824 (2)	C11—C12	1.455 (4)
S2—C7	1.755 (2)	C11—H11A	0.9900
S2—C11	1.814 (2)	C11—H11B	0.9900
N1—C6	1.307 (3)	C12—C13	1.176 (4)
N1—C5	1.368 (3)	C13—H13	0.9500
N2—C7	1.303 (3)		
C2—C3—C4	119.7 (2)	N3—C5—N1	116.0 (2)
C2—C3—Br1	120.6 (2)	N3—C5—C1	123.0 (2)

C4—C3—Br1	119.6 (2)	N1—C5—C1	121.0 (2)
N3—C4—C3	123.8 (2)	N1—C6—C7	122.2 (2)
N3—C4—H4	118.1	N1—C6—S1	120.73 (18)
C3—C4—H4	118.1	C7—C6—S1	117.11 (17)
C2—C3A—C4A	119.7 (2)	N2—C7—C6	121.5 (2)
C2—C3A—H3A	118.6	N2—C7—S2	121.34 (18)
C4A—C3A—H3A	121.6	C6—C7—S2	117.14 (17)
N3—C4A—C3A	123.8 (2)	C9—C8—S1	108.37 (17)
N3—C4A—Br1A	145.9 (4)	C9—C8—H8A	110.0
C3A—C4A—Br1A	90.3 (4)	S1—C8—H8A	110.0
C6—S1—C8	99.78 (11)	C9—C8—H8B	110.0
C7—S2—C11	100.09 (11)	S1—C8—H8B	110.0
C6—N1—C5	116.8 (2)	H8A—C8—H8B	108.4
C7—N2—C1	116.8 (2)	C10—C9—C8	179.0 (3)
C4A—N3—C5	117.2 (2)	C9—C10—H10	180.0
C4—N3—C5	117.2 (2)	C12—C11—S2	113.08 (17)
N2—C1—C2	119.7 (2)	C12—C11—H11A	109.0
N2—C1—C5	121.7 (2)	S2—C11—H11A	109.0
C2—C1—C5	118.5 (2)	C12—C11—H11B	109.0
C3A—C2—C1	117.6 (2)	S2—C11—H11B	109.0
C3—C2—C1	117.6 (2)	H11A—C11—H11B	107.8
C3—C2—H2	121.2	C13—C12—C11	178.6 (3)
C1—C2—H2	121.2	C12—C13—H13	180.0

C2—C3—C4—N3	1.9 (4)	C4—N3—C5—C1	−1.5 (4)
Br1—C3—C4—N3	−176.1 (2)	C6—N1—C5—N3	179.6 (2)
C2—C3A—C4A—N3	1.9 (4)	C6—N1—C5—C1	−0.2 (3)
Br1A—C3A—C4A—N3	179.5 (5)	N2—C1—C5—N3	−179.9 (2)
C2—C3A—C4A—Br1A	−177.6 (4)	C2—C1—C5—N3	1.0 (4)
C3A—Br1A—C4A—N3	−179.2 (7)	N2—C1—C5—N1	−0.1 (4)
C3A—C4A—N3—C5	0.1 (4)	C2—C1—C5—N1	−179.2 (2)
Br1A—C4A—N3—C5	179.2 (7)	C5—N1—C6—C7	−0.1 (3)
C3—C4—N3—C5	0.1 (4)	C5—N1—C6—S1	−179.46 (17)
C7—N2—C1—C2	179.9 (2)	C8—S1—C6—N1	0.2 (2)
C7—N2—C1—C5	0.7 (3)	C8—S1—C6—C7	−179.20 (18)
C4A—C3A—C2—C1	−2.3 (4)	C1—N2—C7—C6	−1.0 (3)
C4—C3—C2—C1	−2.3 (4)	C1—N2—C7—S2	178.35 (17)
Br1—C3—C2—C1	175.62 (18)	N1—C6—C7—N2	0.8 (4)
N2—C1—C2—C3A	−178.1 (2)	S1—C6—C7—N2	−179.84 (18)
C5—C1—C2—C3A	1.0 (4)	N1—C6—C7—S2	−178.63 (18)
N2—C1—C2—C3	−178.1 (2)	S1—C6—C7—S2	0.7 (2)
C5—C1—C2—C3	1.0 (4)	C11—S2—C7—N2	3.2 (2)
C4A—N3—C5—N1	178.7 (2)	C11—S2—C7—C6	−177.38 (18)
C4—N3—C5—N1	178.7 (2)	C6—S1—C8—C9	175.29 (17)
C4A—N3—C5—C1	−1.5 (4)	C7—S2—C11—C12	76.78 (19)