research communications

Crystal structure of 2-{[5-(methylsulfanyl)-4-phenyl-4H-1,2,4-triazol-3-yl]methyl}benzo[d]thiazole

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In the structure of the title compound, $C_{17}H_{14}N_4O_2$, the triazole ring exhibits interplanar angles of 63.86 (2) and 76.96 (2)° with the phenyl and benzothiazole planes, respectively. The C—C—C angle at the methylene group is rather wide at 114.28 (4)°. The packing involves three borderline C—H⋯N contacts, two of which combine to form layers parallel to ac, and a pairing of the triazole rings across an inversion centre [interplanar distance of 3.1852 (2) Å].

1. Chemical context

Benzothiazoles and their derivatives are among the most important heterocyclic compounds in medicinal chemistry and are essential to many natural products and therapeutic preparations (Bonde *et al.*, 2015). The derivatives involve a wide range of structural variants (Rana *et al.*, 2008), and their pharmacological qualities are reflected in the extensive hunt for new therapeutically active compounds (Wang *et al.*, 2009), which represents a rapidly developing research area (Abdallah *et al.*, 2023*a,b*; Ammazzalorso *et al.*, 2020; Gill *et al.*, 2015). In particular, several substances based on benzothiazole derivatives have been adapted and/or further developed for clinical practice to treat a wide range of diseases with great therapeutic efficacy (Huang *et al.*, 2009; Seenaiah *et al.*, 2014).

As part of our development of synthetic methods for the preparation of benzothiazole-based heterocycles and other pharmaceutically interesting heterocycles (Ahmed *et al.*, 2022; Yakout *et al.*, 1999), we recently described the synthesis and biological activity of a series of 2-pyrimidyl- and 2-pyridylbenzothiazole derivatives with encouraging cytotoxic activity (Azzam *et al.* 2020*a,b,c*, 2022*a,b*).
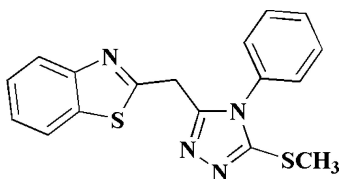
As a continuation of this programme, related to our recent results (Elgemeie *et al.*, 2020, 2022; Metwally *et al.*, 2022*a,b*), the purpose of the present study was to design and synthesize benzothiazolyl-triazole hybrids. The synthesis of our target benzothiazole-2-triazole derivative **5** was achieved by reacting the 2-benzothiazolyl acetohydrazide **1** with phenyl isothiocyanate **2** in the presence of sodium ethoxide, followed by addition of methyl iodide to give **5** in good yield (Fig. 1). The formation of **5** is assumed to proceed *via* initial formation of adduct **4**, with subsequent elimination of water. In order to
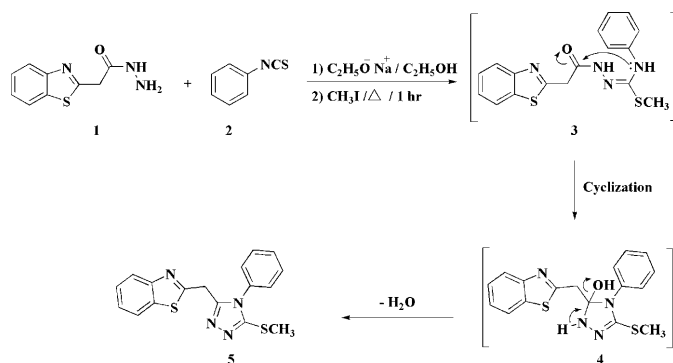
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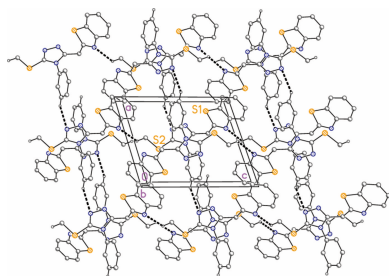
Figure 1
Reaction scheme for the synthesis of **5**.

establish the structure of the product unambiguously, its crystal structure was determined and is reported here.

2. Structural commentary

The structure of compound **5** is shown in Fig. 2. Bond lengths and angles may be generally regarded as normal; *e.g.* the two S2—C bond lengths differ appreciably, reflecting the different hybridizations of C10 and C11. One exception may be the angle C2—C8—C9 at the methylene group, which is rather wide at 114.28 (4)° (see below). A selection, mostly involving the heteroatoms, is presented in Table 1. The triazole ring subtends interplanar angles of 63.86 (2) and 76.96 (2)° with the phenyl and benzothiazole planes, respectively. The intramolecular distance $S1\cdots N1$ is 3.4819 (5) Å, far too long to represent any significant interaction, in contrast to the value of 2.7570 (8) Å that we recently observed for the intramolecular $S\cdots N_{imine}$ contact in N-[3-(benzo[d]thiazol-2-yl)-6-bromo-2H-chromen-2-ylidene]-4-methylbenzenamine (Abdallah *et al.*, 2023*a*).

3. Supramolecular features

The molecular packing displays few significant features. There are three borderline C—H···N interactions (Table 2), two of which (the first and third in Table 2) connect the molecules by
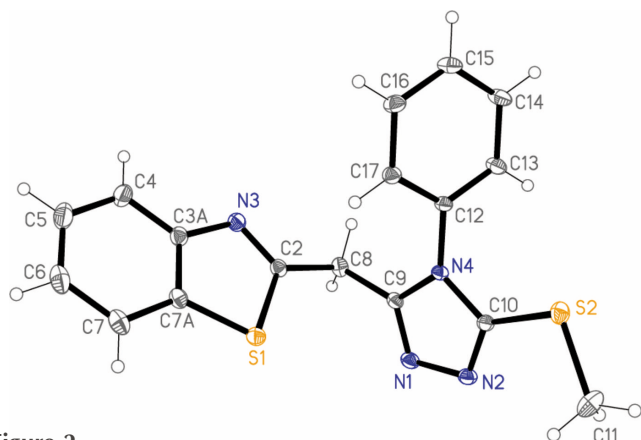
Table 1
Selected geometric parameters (Å, °).

S1—C7*A*	1.7334 (5)	N2—C10	1.3150 (6)
S1—C2	1.7503 (5)	N3—C2	1.2973 (6)
S2—C10	1.7418 (5)	N3—C3*A*	1.3905 (7)
S2—C11	1.8063 (6)	N4—C10	1.3716 (6)
N1—C9	1.3094 (6)	N4—C9	1.3754 (6)
N1—N2	1.3968 (6)		
C7*A*—S1—C2	88.86 (2)	C10—N4—C9	104.30 (4)
C10—S2—C11	98.33 (3)	N3—C2—S1	116.30 (4)
C9—N1—N2	107.60 (4)	C9—C8—C2	114.28 (4)
C10—N2—N1	106.63 (4)	N1—C9—N4	110.51 (4)
C2—N3—C3*A*	110.40 (4)	N2—C10—N4	110.97 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···N3[i]	0.98	2.68	3.3610 (8)	127
C13—H13···N1[ii]	0.95	2.68	3.3609 (6)	129
C14—H14···N2[iii]	0.95	2.67	3.3431 (6)	129

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

translation to form thick layers parallel to the *ac* plane (Fig. 3). The triazole rings are associated in pairs (presumably representing a π–π interaction) *via* the operator $1 - x, -y, 1 - z$, with intercentroid, interplanar and offset distances of 3.3222 (3), 3.1852 (2) and 0.94 Å, respectively. This feature is reinforced by the other C—H···N interaction, which involves the same operator.

4. Database survey

The searches employed the routine ConQuest (Bruno *et al.*, 2002), part of Version 2022.3.0 of the Cambridge Database (Groom *et al.*, 2016).

Only one other structure containing both a triazole and a benzo[*d*]thiazole ring system was found, namely 2-(6-phenyl-7H-1,2,4-triazolo[3,4-*b*]-[1,3,4]thiadiazin-3-yl)-1,3-benzothia-

Figure 2
The molecule of compound **5** in the crystal. Ellipsoids represent 50% probability levels.
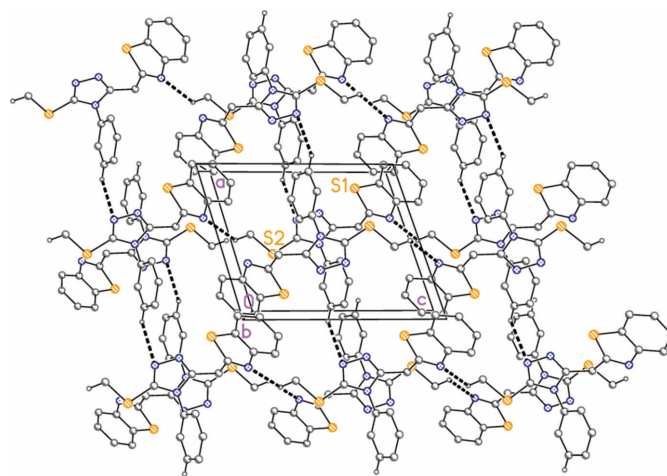

Figure 3
Packing diagram of compound **5**, showing the layer structure parallel to *ac* in the region $y \simeq 0.25$. Thick dashed bonds represent 'weak' C—H···N hydrogen bonds. The labelled atoms indicate the asymmetric unit.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}N_4S_2$
M_r	338.44
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	8.9714 (2), 9.3564 (3), 10.4969 (2)
α, β, γ (°)	94.088 (2), 105.954 (2), 107.393 (2)
V (Å^3)	797.05 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.34
Crystal size (mm)	$0.17 \times 0.12 \times 0.10$
Data collection	
Diffractometer	XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.859, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	102462, 10466, 9289
R_{int}	0.033
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.927
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.028, 0.086, 1.04
No. of reflections	10466
No. of parameters	209
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.66, −0.25

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *XP* (Siemens, 1994).

zole (refcode AZUYEU; Abdel-Aziz *et al.*, 2011). This, however, contains a further heterocycle fused to the triazole ring.

To see if the C—C—C angle at the methylene group of **5** is unusually wide, a search was performed for all structures with two five-membered rings connected across a methylene group; the one restriction was that both of the outer carbon atoms should be three-coordinated. This led (excluding a few clear outliers) to 445 values in the range 106–122°, with a mean value of 114 (5)°. However, restricting one ring to be a C2-substituted thiazole gave only three hits, with four values of 109.6–112.9° for the angle at the methylene groups. These all involved two planar ring systems of the benzo[*d*]thiazole type, but with different heteroatoms in some cases (HANSIB and HANSOH, Dauer *et al.*, 2017; KONTAK, Dauer & Stalke, 2014).

5. Synthesis and crystallization

A mixture of 2-benzothiazolyl acetohydrazide **1** (0.01 mol) and phenyl isothiocyanate **2** (0.01 mol) was stirred for 30 min in ethanol (25 mL) in the presence of sodium ethoxide (0.01 mol). After cooling, methyl iodide (0.015 mol) was added. The reaction mixture was stirred for 30 min at room temperature, then refluxed for 1 h. The resulting precipitate was filtered off, washed with water, dried, and recrystallized from ethanol. The title compound was isolated as a white solid; yield 75%; m.p. 429 K; IR (KBr, cm^{-1}): ν 3053 (Ar—CH), 2928 (aliphatic H), 1594 (C=N); ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.60 (*s*, 3H, SCH$_3$), 4.57 (*s*, 2H, CH$_2$), 7.36–7.50 (*m*, 7H, 5 Ar-H and 2 benzothiazole-H), 7.89 (*d*, J = 8.0 Hz, 1H, benzothiazole-H), 8.01 (*d*, J = 8.0 Hz, 1H, benzothiazole-H); Analysis calculated for $C_{17}H_{14}N_4S_2$ (338.45): C 60.33, H 4.17, N 16.55, S 18.95. Found C 60.66; H 4.15; N 16.40; S 18.90%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The methyl group was included as an idealized rigid group allowed to rotate but not tip (C—H = 0.98 Å, H—C—H = 109.5°). Other hydrogen atoms were included using a riding model starting from calculated positions (C—H$_{aromatic}$ = 0.95 Å, C—H$_{methylene}$ = 0.99 Å). The U(H) values were fixed at $1.5 \times U_{eq}$ of the parent carbon atoms for the methyl group and $1.2 \times U_{eq}$ for other hydrogens.

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supporting information

Crystal structure of 2-{[5-(methylsulfanyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl]methyl}benzo[*d*]thiazole

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Computing details

Data collection: *CrysAlis PRO* 1.171.41.122a (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* 1.171.41.122a (Rigaku OD, 2021); data reduction: *CrysAlis PRO* 1.171.41.122a (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2019/3* (Sheldrick, 2015b); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL2019/3* (Sheldrick, 2015b).

2-{[5-(Methylsulfanyl)-4-phenyl-4*H*-1,2,4-triazol-3-yl]methyl}benzo[*d*]thiazole

Crystal data

$C_{17}H_{14}N_4S_2$	$Z = 2$
$M_r = 338.44$	$F(000) = 352$
Triclinic, $P\bar{1}$	$D_x = 1.410$ Mg m^{-3}
$a = 8.9714$ (2) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.3564$ (3) Å	Cell parameters from 69237 reflections
$c = 10.4969$ (2) Å	$\theta = 2.3–41.4°$
$\alpha = 94.088$ (2)°	$\mu = 0.34$ mm^{-1}
$\beta = 105.954$ (2)°	$T = 100$ K
$\gamma = 107.393$ (2)°	Tablet, colourless
$V = 797.05$ (3) Å^3	$0.17 \times 0.12 \times 0.10$ mm

Data collection

XtaLAB Synergy diffractometer	$T_{min} = 0.859$, $T_{max} = 1.000$
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source	102462 measured reflections
	10466 independent reflections
Mirror monochromator	9289 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0000 pixels mm^{-1}	$R_{int} = 0.033$
ω scans	$\theta_{max} = 41.2°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)	$h = -16\rightarrow16$
	$k = -17\rightarrow17$
	$l = -19\rightarrow19$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: dual
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.086$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.0903P]$
10466 reflections	where $P = (F_o^2 + 2F_c^2)/3$
209 parameters	

$(\Delta/\sigma)_{max} = 0.001$ $\Delta\rho_{min} = -0.25$ e Å^{-3}

$\Delta\rho_{max} = 0.66$ 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.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

- 0.6560 (0.0019) x - 4.9080 (0.0018) y + 9.3027 (0.0011) z = 3.1483 (0.0010)

* -0.0006 (0.0003) C12 * 0.0030 (0.0004) C13 * -0.0029 (0.0004) C14 * 0.0003 (0.0004) C15 * 0.0021 (0.0004) C16 * -0.0019 (0.0003) C17 0.0217 (0.0007) N4

Rms deviation of fitted atoms = 0.0021

2.6765 (0.0019) x + 7.5840 (0.0013) y - 0.9757 (0.0024) z = 2.4430 (0.0013)

Angle to previous plane (with approximate esd) = 63.863 (0.019)

* -0.0001 (0.0003) N1 * 0.0018 (0.0003) N2 * 0.0025 (0.0002) N4 * -0.0014 (0.0003) C9 * -0.0027 (0.0003) C10 -0.0058 (0.0008) C8 -0.0865 (0.0007) C12 0.0346 (0.0007) S2

Rms deviation of fitted atoms = 0.0019

5.3893 (0.0012) x - 6.3624 (0.0008) y + 5.1564 (0.0013) z = 5.5973 (0.0010)

Angle to previous plane (with approximate esd) = 76.957 (0.014)

* -0.0079 (0.0003) S1 * 0.0083 (0.0003) C2 * -0.0011 (0.0004) N3 * 0.0009 (0.0004) C3A * -0.0081 (0.0005) C4 * 0.0025 (0.0005) C5 * 0.0038 (0.0005) C6 * -0.0013 (0.0004) C7 * 0.0028 (0.0004) C7A 0.0979 (0.0006) C8

Rms deviation of fitted atoms = 0.0050

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.86054 (2)	0.48129 (2)	0.77843 (2)	0.01557 (3)
S2	0.40521 (2)	0.21180 (2)	0.21857 (2)	0.01692 (3)
N1	0.69326 (5)	0.14743 (5)	0.54398 (4)	0.01461 (6)
N2	0.64593 (5)	0.14656 (5)	0.40548 (4)	0.01439 (6)
N3	0.65416 (5)	0.41599 (5)	0.91486 (4)	0.01501 (6)
N4	0.47354 (4)	0.21828 (4)	0.48932 (4)	0.01123 (5)
C2	0.68997 (5)	0.36293 (5)	0.81379 (5)	0.01319 (6)
C3A	0.76637 (6)	0.55937 (6)	0.97489 (5)	0.01493 (7)
C4	0.76214 (7)	0.64760 (7)	1.08644 (6)	0.02094 (9)
H4	0.678550	0.611765	1.127062	0.025*
C5	0.88296 (8)	0.78864 (7)	1.13624 (6)	0.02484 (10)
H5	0.882744	0.849356	1.212644	0.030*
C6	1.00541 (8)	0.84304 (7)	1.07564 (7)	0.02362 (10)
H6	1.086509	0.940173	1.111582	0.028*
C7	1.01035 (7)	0.75745 (6)	0.96388 (6)	0.02010 (9)
H7	1.092893	0.794830	0.922535	0.024*
C7A	0.88963 (6)	0.61445 (5)	0.91440 (5)	0.01491 (7)
C8	0.59619 (6)	0.20550 (5)	0.73494 (5)	0.01490 (7)
H8A	0.647569	0.133827	0.778009	0.018*
H8B	0.482421	0.175752	0.739460	0.018*
C9	0.58961 (5)	0.18991 (5)	0.59118 (5)	0.01228 (6)
C10	0.51471 (5)	0.18851 (5)	0.37612 (5)	0.01212 (6)
C11	0.54143 (10)	0.18497 (8)	0.12746 (7)	0.02628 (11)
H11A	0.500730	0.200775	0.034712	0.039*

H11B	0.545540	0.081470	0.127332	0.039*
H11C	0.651920	0.258121	0.170908	0.039*
C12	0.33320 (5)	0.25713 (5)	0.49752 (5)	0.01169 (6)
C13	0.17638 (6)	0.15400 (5)	0.43243 (6)	0.01604 (7)
H13	0.162422	0.059676	0.382357	0.019*
C14	0.04025 (6)	0.19174 (6)	0.44212 (6)	0.01850 (8)
H14	−0.067511	0.123172	0.397683	0.022*
C15	0.06206 (6)	0.32983 (6)	0.51686 (6)	0.01743 (8)
H15	−0.030950	0.354811	0.523584	0.021*
C16	0.21950 (6)	0.43126 (6)	0.58166 (5)	0.01627 (7)
H16	0.233522	0.525098	0.632575	0.020*
C17	0.35680 (6)	0.39572 (5)	0.57216 (5)	0.01364 (7)
H17	0.464502	0.464813	0.615821	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01412 (5)	0.01676 (5)	0.01501 (5)	0.00285 (4)	0.00577 (4)	0.00253 (4)
S2	0.01817 (5)	0.01874 (5)	0.01337 (5)	0.00661 (4)	0.00344 (4)	0.00346 (4)
N1	0.01107 (13)	0.01546 (14)	0.01739 (16)	0.00585 (11)	0.00320 (12)	0.00174 (12)
N2	0.01163 (13)	0.01526 (14)	0.01706 (16)	0.00536 (11)	0.00506 (12)	0.00130 (12)
N3	0.01422 (14)	0.01645 (15)	0.01332 (15)	0.00367 (12)	0.00428 (12)	0.00227 (12)
N4	0.00944 (12)	0.01239 (13)	0.01242 (14)	0.00476 (10)	0.00313 (10)	0.00170 (10)
C2	0.01226 (15)	0.01421 (15)	0.01189 (15)	0.00350 (12)	0.00266 (12)	0.00293 (12)
C3A	0.01476 (16)	0.01592 (16)	0.01294 (16)	0.00514 (13)	0.00257 (13)	0.00182 (13)
C4	0.0226 (2)	0.0228 (2)	0.01640 (19)	0.00840 (18)	0.00479 (17)	−0.00129 (16)
C5	0.0265 (2)	0.0221 (2)	0.0212 (2)	0.00883 (19)	0.00129 (19)	−0.00446 (18)
C6	0.0222 (2)	0.01629 (19)	0.0242 (2)	0.00439 (17)	−0.00227 (18)	−0.00112 (17)
C7	0.01646 (18)	0.01581 (18)	0.0226 (2)	0.00197 (14)	0.00139 (16)	0.00295 (16)
C7A	0.01367 (16)	0.01456 (16)	0.01459 (17)	0.00406 (13)	0.00200 (13)	0.00291 (13)
C8	0.01522 (16)	0.01389 (15)	0.01334 (16)	0.00301 (13)	0.00283 (13)	0.00258 (12)
C9	0.01024 (14)	0.01221 (14)	0.01353 (16)	0.00399 (11)	0.00216 (12)	0.00169 (12)
C10	0.01095 (14)	0.01190 (14)	0.01336 (16)	0.00363 (11)	0.00398 (12)	0.00119 (12)
C11	0.0363 (3)	0.0289 (3)	0.0200 (2)	0.0127 (2)	0.0159 (2)	0.00653 (19)
C12	0.00982 (13)	0.01180 (14)	0.01430 (16)	0.00444 (11)	0.00418 (12)	0.00211 (12)
C13	0.01030 (14)	0.01344 (16)	0.0229 (2)	0.00391 (12)	0.00377 (14)	−0.00030 (14)
C14	0.01035 (15)	0.01583 (17)	0.0290 (2)	0.00453 (13)	0.00582 (15)	0.00189 (16)
C15	0.01381 (16)	0.01674 (17)	0.0259 (2)	0.00773 (14)	0.00937 (16)	0.00506 (15)
C16	0.01628 (17)	0.01471 (16)	0.0206 (2)	0.00720 (14)	0.00803 (15)	0.00189 (14)
C17	0.01255 (15)	0.01250 (15)	0.01612 (17)	0.00444 (12)	0.00489 (13)	0.00105 (12)

Geometric parameters (Å, º)

S1—C7A	1.7334 (5)	C12—C17	1.3928 (6)
S1—C2	1.7503 (5)	C12—C13	1.3940 (6)
S2—C10	1.7418 (5)	C13—C14	1.3955 (7)
S2—C11	1.8063 (6)	C14—C15	1.3939 (7)
N1—C9	1.3094 (6)	C15—C16	1.3917 (7)

N1—N2	1.3968 (6)	C16—C17	1.3948 (6)
N2—C10	1.3150 (6)	C4—H4	0.9500
N3—C2	1.2973 (6)	C5—H5	0.9500
N3—C3A	1.3905 (7)	C6—H6	0.9500
N4—C10	1.3716 (6)	C7—H7	0.9500
N4—C9	1.3754 (6)	C8—H8A	0.9900
N4—C12	1.4330 (5)	C8—H8B	0.9900
C2—C8	1.5050 (7)	C11—H11A	0.9800
C3A—C4	1.3997 (7)	C11—H11B	0.9800
C3A—C7A	1.4084 (7)	C11—H11C	0.9800
C4—C5	1.3873 (9)	C13—H13	0.9500
C5—C6	1.4023 (10)	C14—H14	0.9500
C6—C7	1.3912 (9)	C15—H15	0.9500
C7—C7A	1.3994 (7)	C16—H16	0.9500
C8—C9	1.4887 (7)	C17—H17	0.9500
C7A—S1—C2	88.86 (2)	C16—C15—C14	120.28 (4)
C10—S2—C11	98.33 (3)	C15—C16—C17	120.28 (4)
C9—N1—N2	107.60 (4)	C12—C17—C16	118.83 (4)
C10—N2—N1	106.63 (4)	C5—C4—H4	120.8
C2—N3—C3A	110.40 (4)	C3A—C4—H4	120.8
C10—N4—C9	104.30 (4)	C4—C5—H5	119.5
C10—N4—C12	127.66 (4)	C6—C5—H5	119.5
C9—N4—C12	127.84 (4)	C7—C6—H6	119.4
N3—C2—C8	122.28 (4)	C5—C6—H6	119.4
N3—C2—S1	116.30 (4)	C6—C7—H7	121.1
C8—C2—S1	121.35 (3)	C7A—C7—H7	121.1
N3—C3A—C4	124.68 (5)	C9—C8—H8A	108.7
N3—C3A—C7A	115.00 (4)	C2—C8—H8A	108.7
C4—C3A—C7A	120.32 (5)	C9—C8—H8B	108.7
C5—C4—C3A	118.40 (6)	C2—C8—H8B	108.7
C4—C5—C6	121.08 (6)	H8A—C8—H8B	107.6
C7—C6—C5	121.24 (5)	S2—C11—H11A	109.5
C6—C7—C7A	117.76 (5)	S2—C11—H11B	109.5
C7—C7A—C3A	121.20 (5)	H11A—C11—H11B	109.5
C7—C7A—S1	129.37 (4)	S2—C11—H11C	109.5
C3A—C7A—S1	109.43 (3)	H11A—C11—H11C	109.5
C9—C8—C2	114.28 (4)	H11B—C11—H11C	109.5
N1—C9—N4	110.51 (4)	C12—C13—H13	120.6
N1—C9—C8	124.86 (4)	C14—C13—H13	120.6
N4—C9—C8	124.63 (4)	C15—C14—H14	119.9
N2—C10—N4	110.97 (4)	C13—C14—H14	119.9
N2—C10—S2	126.93 (4)	C16—C15—H15	119.9
N4—C10—S2	122.07 (3)	C14—C15—H15	119.9
C17—C12—C13	121.63 (4)	C15—C16—H16	119.9
C17—C12—N4	119.25 (4)	C17—C16—H16	119.9
C13—C12—N4	119.12 (4)	C12—C17—H17	120.6
C12—C13—C14	118.84 (4)	C16—C17—H17	120.6

C15—C14—C13	120.14 (5)		
C9—N1—N2—C10	−0.19 (5)	C12—N4—C9—N1	175.49 (4)
C3A—N3—C2—C8	175.98 (4)	C10—N4—C9—C8	−179.64 (4)
C3A—N3—C2—S1	−1.04 (5)	C12—N4—C9—C8	−4.54 (7)
C7A—S1—C2—N3	1.07 (4)	C2—C8—C9—N1	93.15 (6)
C7A—S1—C2—C8	−175.98 (4)	C2—C8—C9—N4	−86.82 (5)
C2—N3—C3A—C4	179.97 (5)	N1—N2—C10—N4	0.44 (5)
C2—N3—C3A—C7A	0.43 (6)	N1—N2—C10—S2	178.46 (3)
N3—C3A—C4—C5	179.66 (5)	C9—N4—C10—N2	−0.51 (5)
C7A—C3A—C4—C5	−0.82 (8)	C12—N4—C10—N2	−175.63 (4)
C3A—C4—C5—C6	0.86 (9)	C9—N4—C10—S2	−178.64 (3)
C4—C5—C6—C7	−0.20 (10)	C12—N4—C10—S2	6.24 (6)
C5—C6—C7—C7A	−0.49 (9)	C11—S2—C10—N2	−6.70 (5)
C6—C7—C7A—C3A	0.52 (8)	C11—S2—C10—N4	171.12 (4)
C6—C7—C7A—S1	179.73 (4)	C10—N4—C12—C17	−119.71 (5)
N3—C3A—C7A—C7	179.70 (5)	C9—N4—C12—C17	66.28 (6)
C4—C3A—C7A—C7	0.13 (8)	C10—N4—C12—C13	61.39 (6)
N3—C3A—C7A—S1	0.35 (5)	C9—N4—C12—C13	−112.62 (5)
C4—C3A—C7A—S1	−179.22 (4)	C17—C12—C13—C14	0.38 (8)
C2—S1—C7A—C7	179.99 (5)	N4—C12—C13—C14	179.25 (5)
C2—S1—C7A—C3A	−0.73 (4)	C12—C13—C14—C15	−0.59 (8)
N3—C2—C8—C9	149.86 (5)	C13—C14—C15—C16	0.35 (9)
S1—C2—C8—C9	−33.27 (6)	C14—C15—C16—C17	0.12 (8)
N2—N1—C9—N4	−0.13 (5)	C13—C12—C17—C16	0.08 (7)
N2—N1—C9—C8	179.90 (4)	N4—C12—C17—C16	−178.79 (4)
C10—N4—C9—N1	0.39 (5)	C15—C16—C17—C12	−0.33 (7)

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C11—H11*A*⋯N3ⁱ	0.98	2.68	3.3610 (8)	127
C13—H13⋯N1ⁱⁱ	0.95	2.68	3.3609 (6)	129
C14—H14⋯N2ⁱⁱⁱ	0.95	2.67	3.3431 (6)	129

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*−1, *y*, *z*.