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Crystal structure of potassium [4-amino-5-(benzo[*d*]thiazol-2-yl)-6-(methylsulfanyl)pyrimidin-2-yl]-(phenylsulfonyl)azanide dimethylformamide monosolvate hemihydrate

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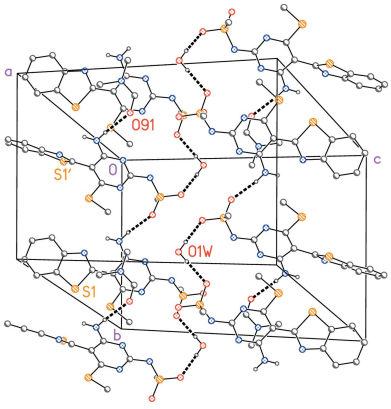
The title compound, $K^+\cdot C_{18}H_{14}N_5O_2S_3^-\cdot C_3H_7NO\cdot 0.5H_2O$, was obtained in a reaction designed to deliver a neutral 2-pyrimidylbenzothiazole. The anion is deprotonated at the sulfonamide nitrogen. The asymmetric unit of the title compound contains two potassium cations, two anions, two molecules of DMF and one of water. The anions display some conformational differences but each contains an intramolecular $N-H\cdots N_{benzothiazole}$ hydrogen bond. The potassium ions both display a highly irregular six-coordination, different for each potassium ion. The anions, together with the DMF and water molecules, are linked by four classical hydrogen bonds to form chains parallel to the *b*-axis direction.



1. Chemical context

Benzothiazoles are versatile heterocyclic biologically active compounds that are common in a variety of pharmaceutical preparations (Azzam *et al.*, 2017*a*,*b*). These compounds are of great importance in the field of medicinal chemistry because of their remarkable pharmacological potential (Keri *et al.*, 2015). Benzothiazole derivatives show a high degree of structural diversity that has proved beneficial in the search for new therapeutic agents (Gill *et al.*, 2015). Research in benzothiazole-based medicinal chemistry has rapidly become an active topic, since numerous benzothiazole-based compounds have been widely used as clinical drugs to treat various types of diseases with high therapeutic potency (Sharma *et al.*, 2013). The medicinal properties associated with benzothiazole-related drugs have encouraged medicinal chemists to synthesize a large number of new therapeutics (Elgemeie & Elghandour, 1990; Elgemeie *et al.*, 2000*a*,*b*). In recent years, 2-pyrimidylbenzothiazoles have appeared as an important pharmacological class in the development of anti-tumor agents (Das *et al.*, 2003); their promising biological profile and synthetic accessibility have been attractive in their design and development as potential chemotherapeutics. In order to access this class of compounds in high yield and to introduce diversity, a variety of new synthetic methods has been invented (Seenaiah *et al.*, 2014). Recently, we have described the syntheses of various antimetabolites starting from heterocyclic and acyclic cyanoketene dithioacetals (Elgemeie *et al.*, 2015, 2016, 2017). As part of this program the reaction of

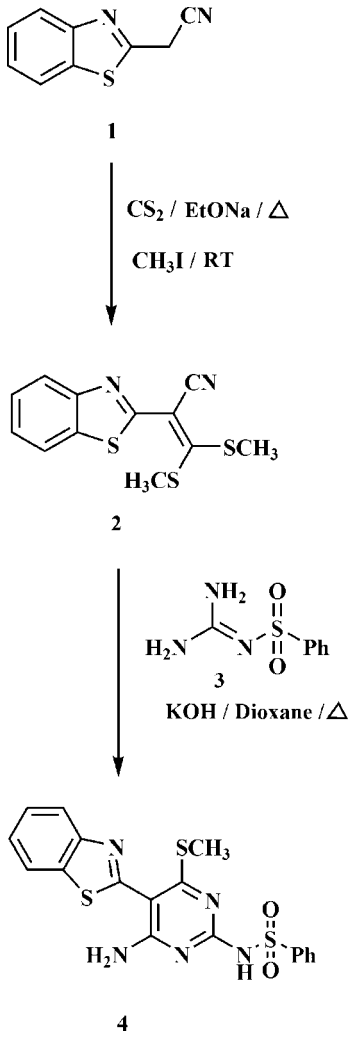
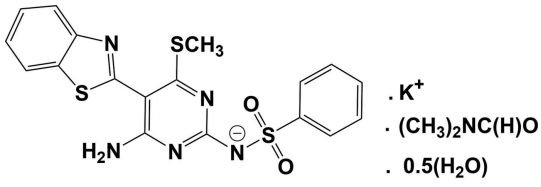


Figure 1
The attempted synthesis of compound **4**.

2-(benzo[*d*]thiazol-2-yl)-3,3-bis(methylthio)acrylonitrile (**2**) with *N*-(diaminomethylene)benzenesulfonamide (**3**) was studied (Fig. 1). The reaction between **2** and **3** in KOH/dioxane gave a product that was crystallized from DMF and identified by X-ray crystallography as the title compound, **5**, rather than the expected neutral 2-pyrimidylbenzothiazole derivative, **4**. Compound **4** appears to be formed, at least in part, on dissolving **5** in deuterated DMSO; ^{1}H NMR measurements showed the free NH proton at δ 11.50 ppm. However, we have still been unable to isolate and crystallize derivative **4**.



(5)

The formation of **5** from the reaction of **2** and **3** is assumed to proceed *via* initial addition of the amino group of **3** to the double bond of **2**, followed by elimination of CH_3SH and cyclization *via* addition of the amino group to the cyano group of benzothiazole to give the product **4**, which separated as its potassium salt **5** in the presence of KOH in the reaction medium. The ^{1}H NMR spectra of the product **4**, formed in part in solution in deuterated DMSO, revealed the presence of a pyrimidine methylthio group at δ = 2.19 ppm and an amino group at δ = 8.49 ppm in solution. Compound **5** and its derivatives showed interesting preclinical antiviral biological results compared to current antiviral drugs and are currently being patented (Elgemeie *et al.*, 2018).

2. Structural commentary

The X-ray crystal structure indicated the exclusive presence of structure **5** in the solid state. The molecular structure of compound **5** is illustrated in Fig. 2. The asymmetric unit contains two potassium cations, two anions of **4** deprotonated at the sulfonamide nitrogen, two molecules of DMF and one of water; it was chosen arbitrarily in an attempt to maximize the number of weak interactions (bonds to potassium, hydrogen bonds) within this unit.

The potassium ions both display a highly irregular six-coordination; all K—N and K—O contacts (Table 1) are < 2.92 Å, and the next longest are > 3.33 Å. The atom K1 is coordinated by the pyrimidine nitrogen atom N2 and the deprotonated sulfonamide nitrogen N5, the sulfonamide oxygen atom O1′ and the water oxygen O1*W* within the asymmetric unit, and by the sulfonamide oxygen atom O2′ and the DMF oxygen O92 at ($-x+1, -y+1, -z+1$). The atom K2 is coordinated by N2′, N5′ and both DMF oxygen atoms within the asymmetric unit, plus O2 at ($-x+1, -y+1, -z+1$) and O1 at ($x, y-1, z$). The angles subtended by the chelating

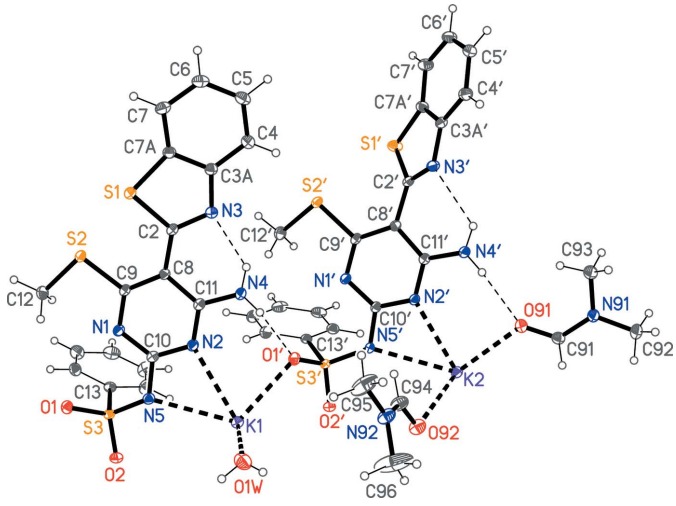


Figure 2
The molecular structure of compound **5**, with the atom labelling (anion 1 has unprimed atom labels, anion 2 has primed atom labels). Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate contacts to the potassium ions (thick) or classical hydrogen bonds (thin). For clarity, the sulfonamide phenyl group is not labelled.

Table 1
Selected geometric parameters (Å, °).

K1—N2	2.8371 (10)	K2—N2′	2.8320 (10)
K1—N5	2.9038 (11)	K2—N5′	2.9133 (10)
K1—O1′	2.6918 (9)	K2—O1^{ii}	2.6846 (10)
K1—O2′^{i}	2.7811 (9)	K2—O2^{i}	2.6782 (9)
K1—O1*W*	2.8991 (13)	K2—O91	2.6594 (10)
K1—O92^{i}	2.6779 (11)	K2—O92	2.8193 (10)
O92^{i}—K1—O1′	122.10 (3)	O91—K2—O1^{ii}	122.24 (3)
O92^{i}—K1—O2′^{i}	89.19 (3)	O2^{i}—K2—O1^{ii}	104.71 (3)
O1′—K1—O2′^{i}	94.53 (3)	O91—K2—O92	116.05 (3)
O92^{i}—K1—N2	117.13 (3)	O2^{i}—K2—O92	74.59 (3)
O1′—K1—N2	72.98 (3)	O1^{ii}—K2—O92	120.48 (3)
O2′^{i}—K1—N2	153.65 (3)	O91—K2—N2′	78.44 (3)
O92^{i}—K1—O1*W*	125.24 (3)	O2^{i}—K2—N2′	145.92 (3)
O1′—K1—O1*W*	105.49 (3)	O1^{ii}—K2—N2′	108.90 (3)
O2′^{i}—K1—O1*W*	59.75 (3)	O92—K2—N2′	92.77 (3)
N2—K1—O1*W*	100.51 (3)	O91—K2—N5′	124.93 (3)
O92^{i}—K1—N5	80.48 (3)	O2^{i}—K2—N5′	145.82 (3)
O1′—K1—N5	116.98 (3)	O1^{ii}—K2—N5′	83.45 (3)
O2′^{i}—K1—N5	147.63 (3)	O92—K2—N5′	72.82 (3)
N2—K1—N5	46.67 (3)	N2′—K2—N5′	46.50 (3)
O1*W*—K1—N5	101.98 (3)	K1^{i}—O92—K2	87.35 (3)
O91—K2—O2^{i}	79.15 (3)		
S1—C2—C8—C9	22.06 (18)	S1′—C2′—C8′—C9′	−42.51 (16)
N1—C10—N5—S3	15.18 (17)	N1′—C10′—N5′—S3′	−15.33 (16)
C13—S3—N5—C10	62.49 (11)	C13′—S3′—N5′—C10′	65.28 (11)

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

anions *via* N2/N5 are particularly narrow. The bridging nature of O92 is shown in Fig. 3.

Each anion displays an intramolecular hydrogen bond (N4—H01···N3 and N4′—H01′···N3′; Table 2), forming an *S*(6) ring motif. The anions display some differences in conformation; the angle between the benzothiazole ring (seven atoms) and the pyrimidine ring plus immediate substituents (ten atoms) is 20.56 (5)° for anion 1 (unprimed atoms) but 42.20 (2)° for anion 2 (primed atoms). Comparing the torsion angles in Table 1, it may be seen that the signs of the torsion angles C9—C8—C2—S1 are different for the two anions [22.06 (18) and −42.51 (16)°]. A molecular fit of the ten

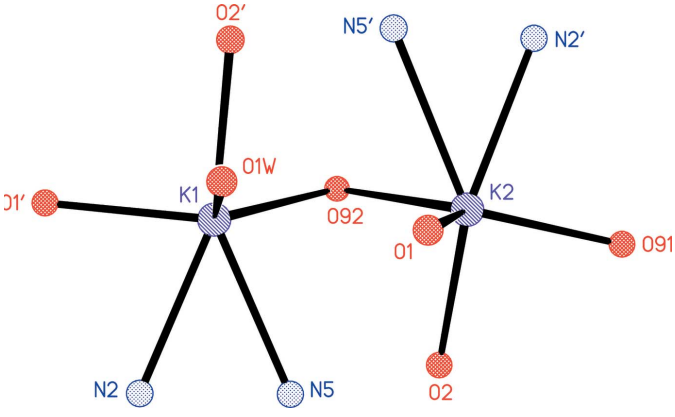


Figure 3
Coordination of the two potassium ions, showing the bridging nature of the DMF oxygen atom O92. Atoms O2′, O91, O92, K2, N2′, N5′ have been transformed to $(-x+1, -y+1, -z+1)$ and O1 to $(-x+1, -y+2, -z+1)$. The K1···K2 distance is 3.7975 (4) Å.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H01···N3	0.85 (2)	2.01 (2)	2.6859 (15)	136 (2)
N4′—H01′···N3′	0.87 (2)	2.26 (2)	2.8781 (15)	129 (2)
N4—H02···O1′	0.87 (2)	2.06 (2)	2.9205 (14)	168 (2)
N4′—H02′···O91	0.847 (19)	2.180 (19)	3.0207 (14)	172 (2)
O1*W*—H03···O2′^{i}	0.81 (2)	2.07 (2)	2.8314 (15)	157 (2)
O1*W*—H04···O1^{iii}	0.82 (3)	2.00 (3)	2.8211 (15)	176 (3)

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

atoms of the pyrimidine ring, inverting one anion, gives an r.m.s. deviation of 0.03 Å (Fig. 4); the benzothiazole rings are then a better fit, but the phenyl rings of the sulfonamide groups then point to opposite sides in the two anions, *cf.* torsion angle C10—N5—S3—C13 is 62.49 (11)°, and 65.28 (11)° in the non-inverted system.

3. Supramolecular features

Classical hydrogen bonds are shown in Table 2. These four hydrogen bonds combined with the contacts at the potassium ions give a highly complex packing pattern. If the potassium ions are omitted, a much more simple pattern emerges; the residues are linked *via* the water molecules to form chains parallel to the *b*-axis direction, two of which are shown in Fig. 5.

4. Database survey

A search of the Cambridge Structural Database (CSD, V5.40, November 2018; Groom *et al.*, 2016) gave 47 hits (including ten duplicated structures) for the fragment consisting of a pyrimidine ring system bearing a two-coordinate, and thus negatively charged, nitrogen substituent at the ring carbon between the two nitrogen atoms, with the nitrogen substituent forming part of a sulfonamide system. The hits included a silver salt (ASULDZ; Cook & Turner, 1975) and a sodium salt (JUBGUI/01; Hannan & Talukdar, 1992; Patel, 1995).

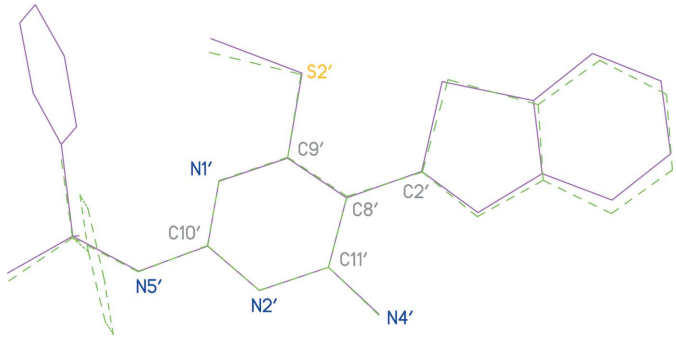


Figure 4
A view of the molecular fit of the two independent anions of compound **5**. Fitted atoms are labelled; anion 1 (inverted from the refined coordinates) is green, anion 2 (primed atoms) is purple.

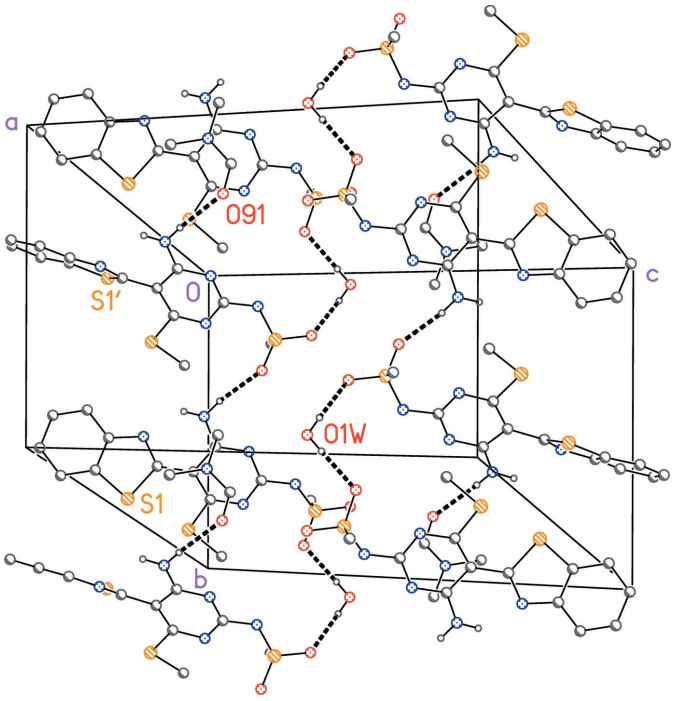


Figure 5
A view normal to plane (101) of the crystal packing of compound **5**. Hydrogen bonds (Table 2) are shown as dashed lines; hydrogen atoms not involved in hydrogen bonding have been omitted for clarity. Also omitted is the DMF molecule based on atom O92 (which does not form any hydrogen bonds). For clarity, the phenyl ring at C13 is reduced to the *ipso* carbon.

5. Synthesis and crystallization

Synthesis of potassium [4-amino-5-(benzo[*d*]thiazol-2-yl)-6-(methylsulfanyl)pyrimidin-2-yl](phenylsulfonyl)azanide dimethylformamide monosolvate hemihydrate (5):

The reaction pathway is illustrated in Fig. 1. 2-(Benzo[*d*]-thiazole-2-yl)-3,3-bis(methylthio)acrylonitrile (**2**) (0.01 mol) was added to a stirred solution of the *N*-(diaminomethyl-ene)benzenesulfonamide (**3**) (0.01 mol) in dry dioxane (20 ml) containing potassium hydroxide (0.01 mol); the reaction mixture was refluxed for 2 h. After completion of the reaction (TLC), the solid precipitate was filtered off, and then recrystallized from DMF/H_2O to give colourless block-like crystals of compound **5**, the potassium salt of compound **4**, in 75% yield (m.p. = 517 K). IR (KBr, cm^{-1}): ν 3431 and 3874 (NH, NH_2). ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.19 (*s*, 3H, SCH_3), 7.32–7.39 (*m*, 4H, 3CH-phenyl, CH benzothiazole), 7.46 (*t*, 1H, J = 8.0 Hz, CH benzothiazole), 7.83–7.85 (*m*, 2H, 2CH-phenyl), 7.92 (*d*, 1H, J = 8.0 Hz, CH benzothiazole), 8.01 (*d*, 1H, J = 8.0 Hz, CH benzothiazole), 8.49 (*s*, *br*, 2H, NH_2), 11.50 (*s*, *br*, 1H, NH).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The NH and OH hydrogen atoms were identified in difference-Fourier maps and refined freely.

Table 3
Experimental details.

Crystal data	
Chemical formula	$K^+ \cdot C_{18}H_{14}N_5O_2S_3^- \cdot C_3H_7NO \cdot 0.5H_2O$
M_r	549.72
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	11.8407 (2), 12.6001 (4), 18.8671 (5)
α, β, γ (°)	90.160 (2), 102.361 (2), 117.933 (3)
V (Å^3)	2411.88 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.52
Crystal size (mm)	0.35 × 0.25 × 0.25
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.994, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	256622, 13912, 11954
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.077, 1.05
No. of reflections	13912
No. of parameters	652
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.40

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015) and *XP* (Siemens, 1994).

Methyl groups were identified from difference-Fourier maps, idealized and refined as rigid groups [C—H = 0.98 Å, H—C—H = 109.5° with U_{iso}(H) = 1.5U_{eq}(C-methyl)], and allowed to rotate but not to tip (AFIX 137). Other hydrogen atoms were included using a riding model starting from calculated positions: C—$H_{aromatic}$ = 0.95 Å with U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

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Crystal structure of potassium [4-amino-5-(benzo[*d*]thiazol-2-yl)-6-(methylsulfanyl)pyrimidin-2-yl](phenylsulfonyl)azanide dimethylformamide monosolvate hemihydrate

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL2017* (Sheldrick, 2015).

Potassium [4-amino-5-(benzo[*d*]thiazol-2-yl)-6-(methylsulfanyl)pyrimidin-2-yl](phenylsulfonyl)azanide dimethylformamide monosolvate hemihydrate

Crystal data

$K^+ \cdot C_{18}H_{14}N_5O_2S_3^- \cdot C_3H_7NO \cdot 0.5H_2O$
$M_r = 549.72$
Triclinic, $P\overline{1}$
$a = 11.8407$ (2) Å
$b = 12.6001$ (4) Å
$c = 18.8671$ (5) Å
$\alpha = 90.160$ (2)°
$\beta = 102.361$ (2)°
$\gamma = 117.933$ (3)°
$V = 2411.88$ (13) Å^3
$Z = 4$
$F(000) = 1140$
$D_x = 1.514$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 60104 reflections
$\theta = 2.4$–30.6°
$\mu = 0.52$ mm^{-1}
$T = 100$ K
Block, colourless
0.35 × 0.25 × 0.25 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed X-ray tube
Detector resolution: 16.1419 pixels mm^{-1}
ω–scan
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.994$, $T_{max} = 1.000$
256622 measured reflections
13912 independent reflections
11954 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -16 \rightarrow 16$
$k = -17 \rightarrow 17$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 1.05$
13912 reflections
652 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 1.360P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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.
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
7.5026 (0.0024) x + 0.9321 (0.0047) y + 8.4090 (0.0051) z = 6.8996 (0.0032)
* -0.0075 (0.0009) C2 * 0.0127 (0.0009) N3 * 0.0119 (0.0012) C3A * -0.0103 (0.0011) C4 * -0.0129 (0.0011) C5 * 0.0036 (0.0011) C6 * 0.0057 (0.0010) C7 * 0.0136 (0.0012) C7A * -0.0168 (0.0007) S1
Rms deviation of fitted atoms = 0.0113
5.7089 (0.0026) x + 5.0746 (0.0027) y + 5.8404 (0.0040) z = 8.9926 (0.0015)
Angle to previous plane (with approximate esd) = 20.556 (0.046)
* 0.0683 (0.0011) C8 * 0.0132 (0.0010) C9 * 0.0105 (0.0010) C10 * -0.0228 (0.0011) C11 * -0.0190 (0.0009) N1 * -0.0234 (0.0010) N2 * 0.1204 (0.0009) C2 * -0.1062 (0.0006) S2 * 0.0646 (0.0008) N5 * -0.1055 (0.0009) N4 -0.1967 (0.0016) C12 -0.2593 (0.0011) S3
Rms deviation of fitted atoms = 0.0689
==========
- 2.2187 (0.0034) x + 11.9323 (0.0012) y - 3.9110 (0.0057) z = 2.1027 (0.0024)
* 0.0421 (0.0009) C2′ * -0.0030 (0.0009) N3′ * -0.0322 (0.0011) C3A′ * -0.0032 (0.0011) C4′ * 0.0107 (0.0011) C5′ * 0.0163 (0.0011) C6′ * 0.0101 (0.0010) C7′ * -0.0308 (0.0011) C7A′ * -0.0099 (0.0007) S1′
Rms deviation of fitted atoms = 0.0220
4.0185 (0.0027) x + 7.7469 (0.0023) y + 2.9794 (0.0039) z = 6.0513 (0.0008)
Angle to previous plane (with approximate esd) = 42.200 (0.021)
* -0.0154 (0.0011) C8′ * 0.0164 (0.0010) C9′ * 0.0066 (0.0010) C10′ * 0.0299 (0.0010) C11′ * 0.0483 (0.0009) N1′ * 0.0253 (0.0009) N2′ * -0.1309 (0.0009) C2′ * 0.0515 (0.0006) S2′ * -0.1005 (0.0008) N5′ * 0.0688 (0.0008) N4′ -0.2532 (0.0017) C12′ 0.1802 (0.0010) S3′
Rms deviation of fitted atoms = 0.0625
==========

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.67977 (4)	1.02828 (3)	0.09802 (2)	0.01751 (7)
S2	0.47162 (3)	1.04245 (3)	0.15477 (2)	0.01496 (6)
S3	0.31676 (3)	0.90940 (3)	0.39554 (2)	0.01143 (6)
C2	0.63692 (12)	0.90552 (11)	0.15096 (6)	0.0128 (2)
C3A	0.73099 (13)	0.85659 (11)	0.07477 (7)	0.0142 (2)
C4	0.77389 (14)	0.78717 (12)	0.04155 (7)	0.0191 (3)
H4	0.762989	0.712529	0.057998	0.023*
C5	0.83241 (14)	0.82984 (13)	−0.01570 (7)	0.0202 (3)
H5	0.862215	0.784025	−0.038767	0.024*
C6	0.84838 (14)	0.93991 (13)	−0.04020 (7)	0.0198 (3)
H6	0.889986	0.967721	−0.079226	0.024*
C7	0.80507 (14)	1.00885 (12)	−0.00895 (7)	0.0189 (3)
H7	0.814762	1.082683	−0.026224	0.023*
C7A	0.74648 (13)	0.96563 (11)	0.04907 (7)	0.0149 (2)

C8	0.57484 (12)	0.89569 (10)	0.21128 (6)	0.0121 (2)
C9	0.50259 (12)	0.95499 (10)	0.22093 (6)	0.0121 (2)
C10	0.46477 (12)	0.87455 (11)	0.32734 (6)	0.0123 (2)
C11	0.57609 (12)	0.81497 (11)	0.26460 (6)	0.0126 (2)
C12	0.37416 (14)	1.08905 (12)	0.19405 (7)	0.0172 (2)
H12A	0.417727	1.120507	0.245597	0.026*
H12B	0.286843	1.019598	0.190301	0.026*
H12C	0.364720	1.152476	0.167707	0.026*
C13	0.17010 (12)	0.82029 (11)	0.32687 (6)	0.0134 (2)
C14	0.11572 (15)	0.69479 (12)	0.32221 (8)	0.0217 (3)
H14	0.159533	0.658842	0.352897	0.026*
C15	−0.00368 (15)	0.62278 (13)	0.27195 (8)	0.0260 (3)
H15	−0.041467	0.537174	0.268056	0.031*
C16	−0.06766 (14)	0.67590 (14)	0.22751 (8)	0.0232 (3)
H16	−0.149850	0.626424	0.193940	0.028*
C17	−0.01210 (14)	0.80064 (13)	0.23196 (8)	0.0219 (3)
H17	−0.055603	0.836490	0.200925	0.026*
C18	0.10750 (13)	0.87374 (12)	0.28186 (7)	0.0172 (2)
H18	0.145806	0.959352	0.285031	0.021*
N1	0.44791 (11)	0.94544 (9)	0.27717 (6)	0.0132 (2)
N2	0.52377 (11)	0.80718 (9)	0.32239 (6)	0.0135 (2)
N3	0.67040 (11)	0.82571 (10)	0.13235 (6)	0.0148 (2)
N4	0.63003 (12)	0.74264 (10)	0.26054 (6)	0.0176 (2)
H02	0.6135 (19)	0.6870 (18)	0.2900 (11)	0.033 (5)*
H01	0.651 (2)	0.7365 (18)	0.2208 (11)	0.034 (5)*
N5	0.41916 (11)	0.86521 (10)	0.38931 (6)	0.0137 (2)
O1	0.35584 (9)	1.03538 (8)	0.38428 (5)	0.01534 (17)
O2	0.28269 (9)	0.87920 (8)	0.46485 (5)	0.01566 (18)
S1′	0.61437 (3)	0.29511 (3)	0.01676 (2)	0.01725 (7)
S2′	0.54376 (3)	0.46946 (3)	0.09428 (2)	0.01721 (7)
S3′	0.46192 (3)	0.42692 (3)	0.35846 (2)	0.01176 (6)
C2′	0.72463 (12)	0.34847 (11)	0.10370 (6)	0.0122 (2)
C3A′	0.85618 (13)	0.34467 (11)	0.03647 (7)	0.0145 (2)
C4′	0.97234 (14)	0.36291 (13)	0.01881 (7)	0.0193 (3)
H4′	1.051620	0.390641	0.055865	0.023*
C5′	0.97023 (15)	0.34001 (13)	−0.05340 (8)	0.0209 (3)
H5′	1.048490	0.351042	−0.065639	0.025*
C6′	0.85444 (15)	0.30083 (12)	−0.10871 (7)	0.0209 (3)
H6′	0.855166	0.285520	−0.157894	0.025*
C7′	0.73941 (15)	0.28421 (12)	−0.09258 (7)	0.0198 (3)
H7′	0.661289	0.259304	−0.130140	0.024*
C7A′	0.74080 (13)	0.30496 (11)	−0.01957 (7)	0.0150 (2)
C8′	0.68045 (12)	0.36129 (10)	0.16870 (6)	0.0115 (2)
C9′	0.59510 (12)	0.40880 (10)	0.17095 (6)	0.0120 (2)
C10′	0.58805 (12)	0.36622 (10)	0.28789 (6)	0.0114 (2)
C11′	0.72036 (12)	0.32086 (10)	0.23520 (6)	0.0117 (2)
C12′	0.41439 (15)	0.48795 (13)	0.11841 (7)	0.0206 (3)
H12D	0.348305	0.410299	0.129017	0.031*

H12E	0.372818	0.515917	0.077628	0.031*
H12F	0.451606	0.547696	0.161728	0.031*
C13′	0.31457 (13)	0.37337 (12)	0.28815 (6)	0.0144 (2)
C14′	0.24643 (13)	0.25133 (12)	0.26169 (7)	0.0163 (2)
H14′	0.280816	0.199034	0.279043	0.020*
C15′	0.12741 (14)	0.20642 (13)	0.20955 (7)	0.0205 (3)
H15′	0.081078	0.123450	0.190146	0.025*
C16′	0.07620 (15)	0.28272 (15)	0.18583 (7)	0.0234 (3)
H16′	−0.006040	0.251404	0.150880	0.028*
C17′	0.14437 (15)	0.40440 (15)	0.21284 (8)	0.0242 (3)
H17′	0.108590	0.456059	0.196406	0.029*
C18′	0.26492 (15)	0.45107 (13)	0.26390 (7)	0.0199 (3)
H18′	0.312684	0.534651	0.281964	0.024*
N1′	0.55003 (11)	0.41385 (9)	0.22932 (5)	0.01266 (19)
N2′	0.67301 (10)	0.32232 (9)	0.29374 (5)	0.01215 (19)
N3′	0.84368 (11)	0.36751 (10)	0.10580 (6)	0.0146 (2)
N4′	0.80664 (11)	0.27784 (10)	0.24374 (6)	0.0154 (2)
H02′	0.8068 (18)	0.2361 (17)	0.2788 (10)	0.026 (5)*
H01′	0.8381 (19)	0.2724 (17)	0.2073 (11)	0.032 (5)*
N5′	0.53703 (11)	0.35582 (9)	0.34781 (5)	0.01244 (19)
O1′	0.53653 (10)	0.55695 (8)	0.35774 (5)	0.01774 (19)
O2′	0.41688 (10)	0.39421 (8)	0.42515 (5)	0.01618 (18)
O1W	0.74945 (12)	0.84359 (11)	0.54810 (6)	0.0277 (2)
H03	0.721 (2)	0.779 (2)	0.5641 (12)	0.043 (6)*
H04	0.722 (3)	0.881 (2)	0.5691 (14)	0.059 (7)*
K1	0.49406 (3)	0.68951 (3)	0.45040 (2)	0.01683 (6)
K2	0.61675 (3)	0.18387 (2)	0.41184 (2)	0.01349 (6)
C91	0.80325 (13)	0.04442 (12)	0.39544 (7)	0.0162 (2)
H91	0.767210	0.011982	0.435682	0.019*
C92	0.90128 (15)	−0.08901 (13)	0.40894 (8)	0.0220 (3)
H92A	0.859007	−0.110674	0.449887	0.033*
H92B	0.996418	−0.057876	0.427120	0.033*
H92C	0.864741	−0.160831	0.373445	0.033*
C93	0.93416 (16)	0.04719 (14)	0.31230 (8)	0.0245 (3)
H93A	0.914558	0.111216	0.294568	0.037*
H93B	0.896673	−0.019652	0.273044	0.037*
H93C	1.029863	0.079505	0.327664	0.037*
N91	0.87702 (12)	0.00353 (10)	0.37388 (6)	0.0171 (2)
O91	0.77808 (10)	0.12169 (9)	0.36692 (5)	0.01859 (19)
C94	0.80107 (14)	0.47812 (13)	0.48372 (8)	0.0227 (3)
H94	0.776435	0.467817	0.431813	0.027*
C95	0.96954 (19)	0.68087 (16)	0.47527 (10)	0.0424 (5)
H95A	0.931121	0.654844	0.422790	0.064*
H95B	1.062670	0.701335	0.486721	0.064*
H95C	0.962128	0.752100	0.488784	0.064*
C96	0.9427 (3)	0.60669 (19)	0.59444 (10)	0.0733 (9)
H96A	1.030708	0.614032	0.610117	0.110*
H96B	0.880906	0.539661	0.615825	0.110*

H96C	0.945776	0.682111	0.610803	0.110*
N92	0.89949 (12)	0.58360 (10)	0.51602 (6)	0.0225 (2)
O92	0.73809 (10)	0.39159 (9)	0.51491 (5)	0.0222 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02517 (18)	0.01570 (14)	0.01810 (14)	0.01219 (13)	0.01195 (12)	0.00747 (11)
S2	0.01847 (16)	0.01588 (14)	0.01479 (13)	0.01093 (12)	0.00581 (11)	0.00621 (11)
S3	0.01119 (14)	0.01133 (12)	0.01105 (12)	0.00464 (11)	0.00318 (10)	0.00208 (9)
C2	0.0127 (6)	0.0121 (5)	0.0126 (5)	0.0052 (5)	0.0028 (4)	0.0032 (4)
C3A	0.0134 (6)	0.0159 (5)	0.0133 (5)	0.0071 (5)	0.0031 (4)	0.0019 (4)
C4	0.0214 (7)	0.0201 (6)	0.0193 (6)	0.0118 (5)	0.0074 (5)	0.0033 (5)
C5	0.0201 (7)	0.0250 (7)	0.0181 (6)	0.0121 (6)	0.0065 (5)	0.0004 (5)
C6	0.0167 (7)	0.0280 (7)	0.0141 (6)	0.0096 (6)	0.0050 (5)	0.0032 (5)
C7	0.0198 (7)	0.0219 (6)	0.0156 (6)	0.0095 (5)	0.0065 (5)	0.0057 (5)
C7A	0.0155 (6)	0.0171 (6)	0.0133 (5)	0.0083 (5)	0.0046 (4)	0.0026 (4)
C8	0.0133 (6)	0.0112 (5)	0.0120 (5)	0.0055 (5)	0.0041 (4)	0.0030 (4)
C9	0.0115 (6)	0.0110 (5)	0.0126 (5)	0.0047 (4)	0.0023 (4)	0.0029 (4)
C10	0.0101 (6)	0.0125 (5)	0.0123 (5)	0.0040 (5)	0.0023 (4)	0.0024 (4)
C11	0.0114 (6)	0.0118 (5)	0.0129 (5)	0.0047 (5)	0.0019 (4)	0.0024 (4)
C12	0.0183 (7)	0.0189 (6)	0.0180 (6)	0.0120 (5)	0.0038 (5)	0.0028 (5)
C13	0.0117 (6)	0.0146 (5)	0.0124 (5)	0.0048 (5)	0.0040 (4)	0.0013 (4)
C14	0.0213 (7)	0.0154 (6)	0.0223 (6)	0.0057 (5)	0.0015 (5)	0.0037 (5)
C15	0.0230 (8)	0.0161 (6)	0.0260 (7)	0.0008 (6)	0.0017 (6)	0.0003 (5)
C16	0.0143 (7)	0.0268 (7)	0.0191 (6)	0.0036 (6)	0.0009 (5)	−0.0039 (5)
C17	0.0184 (7)	0.0274 (7)	0.0200 (6)	0.0130 (6)	−0.0002 (5)	−0.0008 (5)
C18	0.0165 (7)	0.0176 (6)	0.0184 (6)	0.0095 (5)	0.0030 (5)	0.0005 (5)
N1	0.0135 (5)	0.0141 (5)	0.0130 (5)	0.0072 (4)	0.0040 (4)	0.0038 (4)
N2	0.0143 (5)	0.0143 (5)	0.0137 (5)	0.0076 (4)	0.0047 (4)	0.0039 (4)
N3	0.0169 (6)	0.0157 (5)	0.0143 (5)	0.0088 (4)	0.0061 (4)	0.0036 (4)
N4	0.0261 (7)	0.0183 (5)	0.0174 (5)	0.0154 (5)	0.0109 (5)	0.0087 (4)
N5	0.0133 (5)	0.0166 (5)	0.0131 (5)	0.0082 (4)	0.0046 (4)	0.0041 (4)
O1	0.0151 (5)	0.0109 (4)	0.0176 (4)	0.0043 (3)	0.0039 (3)	0.0015 (3)
O2	0.0170 (5)	0.0183 (4)	0.0124 (4)	0.0081 (4)	0.0059 (3)	0.0033 (3)
S1′	0.01307 (16)	0.02409 (16)	0.01137 (13)	0.00726 (13)	0.00081 (11)	−0.00157 (11)
S2′	0.02224 (17)	0.02347 (15)	0.01330 (14)	0.01611 (14)	0.00615 (12)	0.00867 (11)
S3′	0.01608 (15)	0.01188 (13)	0.01004 (12)	0.00854 (11)	0.00399 (10)	0.00284 (9)
C2′	0.0135 (6)	0.0116 (5)	0.0099 (5)	0.0053 (5)	0.0016 (4)	0.0022 (4)
C3A′	0.0174 (6)	0.0149 (5)	0.0126 (5)	0.0084 (5)	0.0047 (5)	0.0037 (4)
C4′	0.0193 (7)	0.0250 (6)	0.0171 (6)	0.0127 (6)	0.0060 (5)	0.0054 (5)
C5′	0.0249 (8)	0.0252 (7)	0.0207 (6)	0.0156 (6)	0.0122 (5)	0.0075 (5)
C6′	0.0290 (8)	0.0218 (6)	0.0150 (6)	0.0131 (6)	0.0093 (5)	0.0030 (5)
C7′	0.0224 (7)	0.0214 (6)	0.0128 (6)	0.0088 (6)	0.0031 (5)	−0.0011 (5)
C7A′	0.0165 (6)	0.0141 (5)	0.0139 (5)	0.0065 (5)	0.0045 (5)	0.0009 (4)
C8′	0.0105 (6)	0.0116 (5)	0.0108 (5)	0.0042 (4)	0.0020 (4)	0.0021 (4)
C9′	0.0119 (6)	0.0099 (5)	0.0121 (5)	0.0042 (4)	0.0016 (4)	0.0030 (4)
C10′	0.0113 (6)	0.0096 (5)	0.0118 (5)	0.0043 (4)	0.0014 (4)	0.0013 (4)

C11′	0.0102 (6)	0.0112 (5)	0.0118 (5)	0.0041 (4)	0.0011 (4)	0.0008 (4)
C12′	0.0236 (7)	0.0284 (7)	0.0179 (6)	0.0194 (6)	0.0041 (5)	0.0058 (5)
C13′	0.0161 (6)	0.0213 (6)	0.0110 (5)	0.0123 (5)	0.0053 (4)	0.0039 (4)
C14′	0.0164 (7)	0.0211 (6)	0.0141 (5)	0.0102 (5)	0.0058 (5)	0.0030 (5)
C15′	0.0165 (7)	0.0272 (7)	0.0152 (6)	0.0075 (6)	0.0064 (5)	0.0014 (5)
C16′	0.0161 (7)	0.0421 (8)	0.0150 (6)	0.0159 (6)	0.0048 (5)	0.0061 (5)
C17′	0.0267 (8)	0.0400 (8)	0.0186 (6)	0.0256 (7)	0.0069 (5)	0.0092 (6)
C18′	0.0254 (8)	0.0259 (7)	0.0161 (6)	0.0185 (6)	0.0055 (5)	0.0043 (5)
N1′	0.0136 (5)	0.0137 (5)	0.0117 (4)	0.0074 (4)	0.0031 (4)	0.0035 (4)
N2′	0.0122 (5)	0.0135 (5)	0.0112 (4)	0.0069 (4)	0.0019 (4)	0.0022 (4)
N3′	0.0145 (5)	0.0179 (5)	0.0118 (5)	0.0080 (4)	0.0039 (4)	0.0034 (4)
N4′	0.0169 (6)	0.0217 (5)	0.0126 (5)	0.0131 (5)	0.0042 (4)	0.0048 (4)
N5′	0.0154 (5)	0.0140 (5)	0.0114 (4)	0.0097 (4)	0.0035 (4)	0.0035 (4)
O1′	0.0255 (5)	0.0119 (4)	0.0171 (4)	0.0094 (4)	0.0065 (4)	0.0032 (3)
O2′	0.0212 (5)	0.0196 (4)	0.0117 (4)	0.0118 (4)	0.0067 (3)	0.0040 (3)
O1W	0.0339 (7)	0.0209 (5)	0.0306 (6)	0.0110 (5)	0.0177 (5)	0.0049 (4)
K1	0.02118 (15)	0.01917 (13)	0.01416 (12)	0.01203 (11)	0.00636 (10)	0.00500 (9)
K2	0.01341 (13)	0.01430 (12)	0.01346 (11)	0.00694 (10)	0.00394 (9)	0.00372 (9)
C91	0.0155 (6)	0.0176 (6)	0.0155 (5)	0.0076 (5)	0.0047 (5)	0.0019 (4)
C92	0.0273 (8)	0.0219 (6)	0.0239 (7)	0.0167 (6)	0.0081 (6)	0.0079 (5)
C93	0.0295 (8)	0.0312 (7)	0.0257 (7)	0.0208 (7)	0.0165 (6)	0.0128 (6)
N91	0.0193 (6)	0.0188 (5)	0.0182 (5)	0.0118 (5)	0.0077 (4)	0.0064 (4)
O91	0.0206 (5)	0.0208 (5)	0.0190 (4)	0.0130 (4)	0.0062 (4)	0.0039 (4)
C94	0.0196 (7)	0.0230 (7)	0.0179 (6)	0.0054 (6)	0.0012 (5)	0.0036 (5)
C95	0.0359 (10)	0.0305 (9)	0.0324 (9)	−0.0041 (8)	0.0014 (7)	0.0163 (7)
C96	0.097 (2)	0.0295 (9)	0.0224 (9)	−0.0215 (11)	0.0030 (10)	−0.0015 (7)
N92	0.0224 (6)	0.0163 (5)	0.0193 (5)	0.0029 (5)	0.0023 (5)	0.0050 (4)
O92	0.0209 (5)	0.0163 (4)	0.0219 (5)	0.0036 (4)	0.0037 (4)	0.0033 (4)

Geometric parameters (Å, º)

S1—C7A	1.7299 (13)	S3′—N5′	1.5672 (10)
S1—C2	1.7716 (12)	S3′—C13′	1.7778 (13)
S2—C9	1.7600 (12)	C2′—N3′	1.3058 (17)
S2—C12	1.7957 (13)	C2′—C8′	1.4685 (16)
S3—O2	1.4500 (9)	C3A′—N3′	1.3915 (15)
S3—O1	1.4611 (9)	C3A′—C4′	1.3986 (19)
S3—N5	1.5770 (11)	C3A′—C7A′	1.4046 (18)
S3—C13	1.7767 (13)	C4′—C5′	1.3843 (18)
C2—N3	1.3126 (16)	C4′—H4′	0.9500
C2—C8	1.4575 (16)	C5′—C6′	1.401 (2)
C3A—N3	1.3859 (16)	C5′—H5′	0.9500
C3A—C7A	1.4008 (17)	C6′—C7′	1.379 (2)
C3A—C4	1.4020 (18)	C6′—H6′	0.9500
C4—C5	1.3822 (19)	C7′—C7A′	1.3964 (17)
C4—H4	0.9500	C7′—H7′	0.9500
C5—C6	1.403 (2)	C8′—C9′	1.4024 (17)
C5—H5	0.9500	C8′—C11′	1.4256 (16)

C6—C7	1.3818 (19)	C9′—N1′	1.3360 (15)
C6—H6	0.9500	C10′—N2′	1.3432 (15)
C7—C7A	1.3966 (17)	C10′—N1′	1.3519 (15)
C7—H7	0.9500	C10′—N5′	1.3708 (15)
C8—C9	1.4100 (17)	C11′—N2′	1.3451 (15)
C8—C11	1.4354 (16)	C11′—N4′	1.3462 (16)
C9—N1	1.3346 (15)	C12′—H12D	0.9800
C10—N2	1.3419 (16)	C12′—H12E	0.9800
C10—N1	1.3507 (15)	C12′—H12F	0.9800
C10—N5	1.3726 (15)	C13′—C14′	1.3877 (18)
C11—N4	1.3454 (16)	C13′—C18′	1.3929 (17)
C11—N2	1.3474 (15)	C14′—C15′	1.3893 (19)
C12—H12A	0.9800	C14′—H14′	0.9500
C12—H12B	0.9800	C15′—C16′	1.387 (2)
C12—H12C	0.9800	C15′—H15′	0.9500
C13—C18	1.3877 (17)	C16′—C17′	1.386 (2)
C13—C14	1.3943 (18)	C16′—H16′	0.9500
C14—C15	1.393 (2)	C17′—C18′	1.390 (2)
C14—H14	0.9500	C17′—H17′	0.9500
C15—C16	1.390 (2)	C18′—H18′	0.9500
C15—H15	0.9500	N4′—H02′	0.847 (19)
C16—C17	1.385 (2)	N4′—H01′	0.87 (2)
C16—H16	0.9500	O1W—H03	0.81 (2)
C17—C18	1.3938 (19)	O1W—H04	0.82 (3)
C17—H17	0.9500	C91—O91	1.2380 (15)
C18—H18	0.9500	C91—N91	1.3291 (17)
K1—N2	2.8371 (10)	C91—H91	0.9500
K1—N5	2.9038 (11)	C92—N91	1.4548 (16)
K1—O1′	2.6918 (9)	C92—H92A	0.9800
K1—O2′^{i}	2.7811 (9)	C92—H92B	0.9800
K1—O1W	2.8991 (13)	C92—H92C	0.9800
K1—O92^{i}	2.6779 (11)	C93—N91	1.4497 (17)
K2—N2′	2.8320 (10)	C93—H93A	0.9800
K2—N5′	2.9133 (10)	C93—H93B	0.9800
K2—O1^{ii}	2.6846 (10)	C93—H93C	0.9800
K2—O2^{i}	2.6782 (9)	C94—O92	1.2333 (17)
K2—O91	2.6594 (10)	C94—N92	1.3177 (18)
K2—O92	2.8193 (10)	C94—H94	0.9500
N4—H02	0.87 (2)	C95—N92	1.4516 (19)
N4—H01	0.85 (2)	C95—H95A	0.9800
S1′—C7A′	1.7299 (13)	C95—H95B	0.9800
S1′—C2′	1.7612 (12)	C95—H95C	0.9800
S2′—C9′	1.7639 (12)	C96—N92	1.439 (2)
S2′—C12′	1.8002 (14)	C96—H96A	0.9800
S3′—O1′	1.4541 (9)	C96—H96B	0.9800
S3′—O2′	1.4566 (9)	C96—H96C	0.9800

C7A—S1—C2	89.78 (6)	N2′—C11′—N4′	115.39 (10)

C9—S2—C12	100.78 (6)	N2′—C11′—C8′	121.93 (11)
O2—S3—O1	113.35 (5)	N4′—C11′—C8′	122.68 (11)
O2—S3—N5	106.98 (5)	S2′—C12′—H12D	109.5
O1—S3—N5	116.05 (6)	S2′—C12′—H12E	109.5
O2—S3—C13	106.02 (6)	H12D—C12′—H12E	109.5
O1—S3—C13	106.14 (6)	S2′—C12′—H12F	109.5
N5—S3—C13	107.73 (6)	H12D—C12′—H12F	109.5
N3—C2—C8	122.89 (11)	H12E—C12′—H12F	109.5
N3—C2—S1	113.58 (9)	C14′—C13′—C18′	121.11 (12)
C8—C2—S1	123.50 (9)	C14′—C13′—S3′	118.40 (9)
N3—C3A—C7A	114.97 (11)	C18′—C13′—S3′	120.36 (10)
N3—C3A—C4	125.16 (11)	C13′—C14′—C15′	119.30 (12)
C7A—C3A—C4	119.86 (12)	C13′—C14′—H14′	120.3
C5—C4—C3A	118.46 (12)	C15′—C14′—H14′	120.3
C5—C4—H4	120.8	C16′—C15′—C14′	120.01 (13)
C3A—C4—H4	120.8	C16′—C15′—H15′	120.0
C4—C5—C6	120.89 (13)	C14′—C15′—H15′	120.0
C4—C5—H5	119.6	C17′—C16′—C15′	120.38 (13)
C6—C5—H5	119.6	C17′—C16′—H16′	119.8
C7—C6—C5	121.59 (12)	C15′—C16′—H16′	119.8
C7—C6—H6	119.2	C16′—C17′—C18′	120.21 (13)
C5—C6—H6	119.2	C16′—C17′—H17′	119.9
C6—C7—C7A	117.32 (12)	C18′—C17′—H17′	119.9
C6—C7—H7	121.3	C17′—C18′—C13′	118.96 (13)
C7A—C7—H7	121.3	C17′—C18′—H18′	120.5
C7—C7A—C3A	121.87 (12)	C13′—C18′—H18′	120.5
C7—C7A—S1	128.54 (10)	C9′—N1′—C10′	116.17 (10)
C3A—C7A—S1	109.57 (9)	C10′—N2′—C11′	117.31 (10)
C9—C8—C11	113.91 (11)	C10′—N2′—K2	101.07 (7)
C9—C8—C2	125.26 (10)	C11′—N2′—K2	136.87 (8)
C11—C8—C2	120.71 (11)	C2′—N3′—C3A′	111.15 (10)
N1—C9—C8	124.03 (11)	C11′—N4′—H02′	116.1 (13)
N1—C9—S2	115.19 (9)	C11′—N4′—H01′	119.3 (13)
C8—C9—S2	120.71 (9)	H02′—N4′—H01′	121.2 (18)
N2—C10—N1	125.23 (11)	C10′—N5′—S3′	120.32 (8)
N2—C10—N5	113.88 (10)	C10′—N5′—K2	96.61 (7)
N1—C10—N5	120.89 (11)	S3′—N5′—K2	143.06 (5)
N4—C11—N2	115.53 (11)	S3′—O1′—K1	114.51 (5)
N4—C11—C8	122.42 (11)	K1—O1W—H03	74.2 (16)
N2—C11—C8	122.05 (11)	K1—O1W—H04	93.9 (18)
S2—C12—H12A	109.5	H03—O1W—H04	103 (2)
S2—C12—H12B	109.5	O92^{i}—K1—O1′	122.10 (3)
H12A—C12—H12B	109.5	O92^{i}—K1—O2′^{i}	89.19 (3)
S2—C12—H12C	109.5	O1′—K1—O2′^{i}	94.53 (3)
H12A—C12—H12C	109.5	O92^{i}—K1—N2	117.13 (3)
H12B—C12—H12C	109.5	O1′—K1—N2	72.98 (3)
C18—C13—C14	120.90 (12)	O2′^{i}—K1—N2	153.65 (3)
C18—C13—S3	120.94 (10)	O92^{i}—K1—O1W	125.24 (3)

C14—C13—S3	118.07 (10)	O1′—K1—O1W	105.49 (3)
C15—C14—C13	119.14 (13)	O2′^{i}—K1—O1W	59.75 (3)
C15—C14—H14	120.4	N2—K1—O1W	100.51 (3)
C13—C14—H14	120.4	O92^{i}—K1—N5	80.48 (3)
C16—C15—C14	120.15 (13)	O1′—K1—N5	116.98 (3)
C16—C15—H15	119.9	O2′^{i}—K1—N5	147.63 (3)
C14—C15—H15	119.9	N2—K1—N5	46.67 (3)
C17—C16—C15	120.28 (13)	O1W—K1—N5	101.98 (3)
C17—C16—H16	119.9	O91—K2—O2^{i}	79.15 (3)
C15—C16—H16	119.9	O91—K2—O1^{ii}	122.24 (3)
C16—C17—C18	120.15 (13)	O2^{i}—K2—O1^{ii}	104.71 (3)
C16—C17—H17	119.9	O91—K2—O92	116.05 (3)
C18—C17—H17	119.9	O2^{i}—K2—O92	74.59 (3)
C13—C18—C17	119.37 (12)	O1^{ii}—K2—O92	120.48 (3)
C13—C18—H18	120.3	O91—K2—N2′	78.44 (3)
C17—C18—H18	120.3	O2^{i}—K2—N2′	145.92 (3)
C9—N1—C10	116.76 (10)	O1^{ii}—K2—N2′	108.90 (3)
C10—N2—C11	117.63 (10)	O92—K2—N2′	92.77 (3)
C10—N2—K1	101.67 (7)	O91—K2—N5′	124.93 (3)
C11—N2—K1	140.70 (8)	O2^{i}—K2—N5′	145.82 (3)
C2—N3—C3A	112.08 (10)	O1^{ii}—K2—N5′	83.45 (3)
C11—N4—H02	116.3 (13)	O92—K2—N5′	72.82 (3)
C11—N4—H01	116.8 (13)	N2′—K2—N5′	46.50 (3)
H02—N4—H01	122.6 (18)	O91—C91—N91	124.77 (12)
C10—N5—S3	121.03 (9)	O91—C91—H91	117.6
C10—N5—K1	97.74 (7)	N91—C91—H91	117.6
S3—N5—K1	137.67 (6)	N91—C92—H92A	109.5
S3—O1—K2^{iii}	115.26 (5)	N91—C92—H92B	109.5
S3—O2—K2^{i}	136.13 (5)	H92A—C92—H92B	109.5
C7A′—S1′—C2′	89.38 (6)	N91—C92—H92C	109.5
C9′—S2′—C12′	101.82 (6)	H92A—C92—H92C	109.5
O1′—S3′—O2′	113.04 (5)	H92B—C92—H92C	109.5
O1′—S3′—N5′	114.63 (6)	N91—C93—H93A	109.5
O2′—S3′—N5′	107.06 (5)	N91—C93—H93B	109.5
O1′—S3′—C13′	107.07 (6)	H93A—C93—H93B	109.5
O2′—S3′—C13′	104.46 (6)	N91—C93—H93C	109.5
N5′—S3′—C13′	110.11 (6)	H93A—C93—H93C	109.5
N3′—C2′—C8′	123.71 (11)	H93B—C93—H93C	109.5
N3′—C2′—S1′	114.91 (9)	C91—N91—C93	121.04 (11)
C8′—C2′—S1′	121.23 (9)	C91—N91—C92	122.18 (11)
N3′—C3A′—C4′	125.82 (12)	C93—N91—C92	116.75 (11)
N3′—C3A′—C7A′	114.92 (11)	C91—O91—K2	120.87 (8)
C4′—C3A′—C7A′	119.19 (11)	O92—C94—N92	125.77 (13)
C5′—C4′—C3A′	119.11 (13)	O92—C94—K2	52.85 (7)
C5′—C4′—H4′	120.4	N92—C94—K2	163.54 (11)
C3A′—C4′—H4′	120.4	O92—C94—H94	117.1
C4′—C5′—C6′	121.01 (13)	N92—C94—H94	117.1
C4′—C5′—H5′	119.5	K2—C94—H94	67.1

C6′—C5′—H5′	119.5	N92—C95—H95A	109.5
C7′—C6′—C5′	120.77 (12)	N92—C95—H95B	109.5
C7′—C6′—H6′	119.6	H95A—C95—H95B	109.5
C5′—C6′—H6′	119.6	N92—C95—H95C	109.5
C6′—C7′—C7A′	118.25 (13)	H95A—C95—H95C	109.5
C6′—C7′—H7′	120.9	H95B—C95—H95C	109.5
C7A′—C7′—H7′	120.9	N92—C96—H96A	109.5
C7′—C7A′—C3A′	121.65 (12)	N92—C96—H96B	109.5
C7′—C7A′—S1′	128.70 (11)	H96A—C96—H96B	109.5
C3A′—C7A′—S1′	109.58 (9)	N92—C96—H96C	109.5
C9′—C8′—C11′	114.77 (11)	H96A—C96—H96C	109.5
C9′—C8′—C2′	124.58 (10)	H96B—C96—H96C	109.5
C11′—C8′—C2′	120.62 (11)	C94—N92—C96	120.61 (13)
N1′—C9′—C8′	123.92 (11)	C94—N92—C95	122.44 (13)
N1′—C9′—S2′	116.05 (9)	C96—N92—C95	116.95 (14)
C8′—C9′—S2′	120.02 (9)	C94—O92—K1^{i}	132.77 (10)
N2′—C10′—N1′	125.70 (11)	C94—O92—K2	106.74 (9)
N2′—C10′—N5′	113.44 (10)	K1^{i}—O92—K2	87.35 (3)
N1′—C10′—N5′	120.83 (11)		

C7A—S1—C2—N3	−0.17 (11)	C3A′—C4′—C5′—C6′	1.0 (2)
C7A—S1—C2—C8	177.68 (11)	C4′—C5′—C6′—C7′	0.1 (2)
N3—C3A—C4—C5	179.77 (13)	C5′—C6′—C7′—C7A′	−1.4 (2)
C7A—C3A—C4—C5	0.8 (2)	C6′—C7′—C7A′—C3A′	1.59 (19)
C3A—C4—C5—C6	−0.1 (2)	C6′—C7′—C7A′—S1′	178.38 (11)
C4—C5—C6—C7	−0.8 (2)	N3′—C3A′—C7A′—C7′	176.71 (12)
C5—C6—C7—C7A	1.1 (2)	C4′—C3A′—C7A′—C7′	−0.55 (19)
C6—C7—C7A—C3A	−0.3 (2)	N3′—C3A′—C7A′—S1′	−0.63 (14)
C6—C7—C7A—S1	−178.52 (11)	C4′—C3A′—C7A′—S1′	−177.89 (10)
N3—C3A—C7A—C7	−179.64 (12)	C2′—S1′—C7A′—C7′	−175.59 (13)
C4—C3A—C7A—C7	−0.6 (2)	C2′—S1′—C7A′—C3A′	1.51 (9)
N3—C3A—C7A—S1	−1.16 (14)	N3′—C2′—C8′—C9′	142.01 (13)
C4—C3A—C7A—S1	177.90 (11)	S1′—C2′—C8′—C9′	−42.51 (16)
C2—S1—C7A—C7	179.08 (13)	N3′—C2′—C8′—C11′	−40.08 (17)
C2—S1—C7A—C3A	0.73 (10)	S1′—C2′—C8′—C11′	135.40 (10)
N3—C2—C8—C9	−160.28 (13)	C11′—C8′—C9′—N1′	−1.83 (17)
S1—C2—C8—C9	22.06 (18)	C2′—C8′—C9′—N1′	176.19 (11)
N3—C2—C8—C11	15.40 (19)	C11′—C8′—C9′—S2′	176.82 (9)
S1—C2—C8—C11	−162.25 (10)	C2′—C8′—C9′—S2′	−5.15 (17)
C11—C8—C9—N1	4.82 (18)	C12′—S2′—C9′—N1′	−12.29 (11)
C2—C8—C9—N1	−179.23 (12)	C12′—S2′—C9′—C8′	168.96 (10)
C11—C8—C9—S2	−171.83 (9)	C9′—C8′—C11′—N2′	3.63 (17)
C2—C8—C9—S2	4.12 (18)	C2′—C8′—C11′—N2′	−174.47 (11)
C12—S2—C9—N1	1.16 (11)	C9′—C8′—C11′—N4′	−176.93 (11)
C12—S2—C9—C8	178.09 (10)	C2′—C8′—C11′—N4′	4.96 (18)
C9—C8—C11—N4	174.05 (12)	O1′—S3′—C13′—C14′	159.94 (10)
C2—C8—C11—N4	−2.09 (19)	O2′—S3′—C13′—C14′	−79.93 (11)
C9—C8—C11—N2	−6.32 (17)	N5′—S3′—C13′—C14′	34.72 (12)

C2—C8—C11—N2	177.53 (11)	O1′—S3′—C13′—C18′	−24.15 (12)
O2—S3—C13—C18	113.30 (11)	O2′—S3′—C13′—C18′	95.97 (11)
O1—S3—C13—C18	−7.52 (12)	N5′—S3′—C13′—C18′	−149.37 (10)
N5—S3—C13—C18	−132.44 (11)	C18′—C13′—C14′—C15′	0.69 (19)
O2—S3—C13—C14	−63.18 (12)	S3′—C13′—C14′—C15′	176.57 (10)
O1—S3—C13—C14	175.99 (10)	C13′—C14′—C15′—C16′	−1.62 (19)
N5—S3—C13—C14	51.07 (12)	C14′—C15′—C16′—C17′	1.2 (2)
C18—C13—C14—C15	−0.6 (2)	C15′—C16′—C17′—C18′	0.1 (2)
S3—C13—C14—C15	175.93 (11)	C16′—C17′—C18′—C13′	−1.0 (2)
C13—C14—C15—C16	−0.4 (2)	C14′—C13′—C18′—C17′	0.6 (2)
C14—C15—C16—C17	1.1 (2)	S3′—C13′—C18′—C17′	−175.16 (10)
C15—C16—C17—C18	−1.0 (2)	C8′—C9′—N1′—C10′	−2.00 (18)
C14—C13—C18—C17	0.7 (2)	S2′—C9′—N1′—C10′	179.30 (9)
S3—C13—C18—C17	−175.65 (10)	N2′—C10′—N1′—C9′	4.65 (18)
C16—C17—C18—C13	0.0 (2)	N5′—C10′—N1′—C9′	−173.44 (11)
C8—C9—N1—C10	0.33 (18)	N1′—C10′—N2′—C11′	−2.95 (18)
S2—C9—N1—C10	177.15 (9)	N5′—C10′—N2′—C11′	175.27 (10)
N2—C10—N1—C9	−4.84 (18)	N1′—C10′—N2′—K2	−162.67 (10)
N5—C10—N1—C9	175.93 (11)	N5′—C10′—N2′—K2	15.55 (11)
N1—C10—N2—C11	3.35 (19)	N4′—C11′—N2′—C10′	179.06 (11)
N5—C10—N2—C11	−177.38 (11)	C8′—C11′—N2′—C10′	−1.46 (17)
N1—C10—N2—K1	−177.35 (11)	N4′—C11′—N2′—K2	−30.78 (17)
N5—C10—N2—K1	1.93 (12)	C8′—C11′—N2′—K2	148.69 (9)
N4—C11—N2—C10	−177.73 (11)	C8′—C2′—N3′—C3A′	178.01 (11)
C8—C11—N2—C10	2.63 (18)	S1′—C2′—N3′—C3A′	2.26 (13)
N4—C11—N2—K1	3.35 (19)	C4′—C3A′—N3′—C2′	176.01 (12)
C8—C11—N2—K1	−176.30 (9)	C7A′—C3A′—N3′—C2′	−1.04 (15)
C8—C2—N3—C3A	−178.31 (11)	N2′—C10′—N5′—S3′	166.36 (9)
S1—C2—N3—C3A	−0.45 (14)	N1′—C10′—N5′—S3′	−15.33 (16)
C7A—C3A—N3—C2	1.06 (16)	N2′—C10′—N5′—K2	−14.92 (10)
C4—C3A—N3—C2	−177.94 (13)	N1′—C10′—N5′—K2	163.39 (10)
N2—C10—N5—S3	−164.13 (9)	O1′—S3′—N5′—C10′	−55.50 (11)
N1—C10—N5—S3	15.18 (17)	O2′—S3′—N5′—C10′	178.27 (9)
N2—C10—N5—K1	−1.86 (11)	C13′—S3′—N5′—C10′	65.28 (11)
N1—C10—N5—K1	177.45 (10)	O1′—S3′—N5′—K2	126.62 (9)
O2—S3—N5—C10	176.11 (10)	O2′—S3′—N5′—K2	0.38 (11)
O1—S3—N5—C10	−56.26 (12)	C13′—S3′—N5′—K2	−112.60 (9)
C13—S3—N5—C10	62.49 (11)	O2′—S3′—O1′—K1	−20.89 (7)
O2—S3—N5—K1	22.74 (10)	N5′—S3′—O1′—K1	−143.97 (5)
O1—S3—N5—K1	150.37 (7)	C13′—S3′—O1′—K1	93.58 (6)
C13—S3—N5—K1	−90.88 (9)	O91—C91—N91—C93	−0.8 (2)
O2—S3—O1—K2^{iii}	99.65 (6)	O91—C91—N91—C92	−178.96 (13)
N5—S3—O1—K2^{iii}	−24.76 (7)	N91—C91—O91—K2	176.30 (10)
C13—S3—O1—K2^{iii}	−144.38 (5)	O92—C94—N92—C96	−0.2 (3)
O1—S3—O2—K2^{i}	−113.35 (8)	K2—C94—N92—C96	−79.3 (4)
N5—S3—O2—K2^{i}	15.85 (9)	O92—C94—N92—C95	179.47 (17)
C13—S3—O2—K2^{i}	130.61 (7)	K2—C94—N92—C95	100.3 (4)
C7A′—S1′—C2′—N3′	−2.26 (10)	N92—C94—O92—K1^{i}	98.16 (17)

C7A′—S1′—C2′—C8′	−178.12 (10)	K2—C94—O92—K1^{i}	−102.27 (11)
N3′—C3A′—C4′—C5′	−177.66 (12)	N92—C94—O92—K2	−159.57 (14)
C7A′—C3A′—C4′—C5′	−0.73 (19)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H01···N3	0.85 (2)	2.01 (2)	2.6859 (15)	136.0 (18)
N4′—H01′···N3′	0.87 (2)	2.26 (2)	2.8781 (15)	128.5 (16)
N4—H02···O1′	0.87 (2)	2.06 (2)	2.9205 (14)	167.5 (18)
N4′—H02′···O91	0.847 (19)	2.180 (19)	3.0207 (14)	172.0 (17)
O1*W*—H03···O2′^{i}	0.81 (2)	2.07 (2)	2.8314 (15)	157 (2)
O1*W*—H04···O1^{iv}	0.82 (3)	2.00 (3)	2.8211 (15)	176 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+2, −*z*+1.