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Crystal structures of five 6-mercaptopurine derivatives

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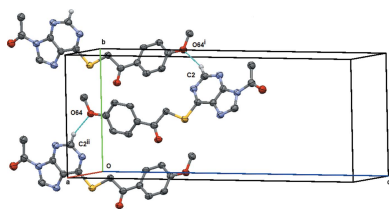
The crystal structures of five 6-mercaptopurine derivatives, *viz.* 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(3-methoxyphenyl)ethan-1-one (**1**), C₁₆H₁₄N₄O₃S, 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-methoxyphenyl)ethan-1-one (**2**), C₁₆H₁₄N₄O₃S, 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-chlorophenyl)ethan-1-one (**3**), C₁₅H₁₁ClN₄O₂S, 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-bromophenyl)ethan-1-one (**4**), C₁₅H₁₁BrN₄O₂S, and 1-(3-methoxyphenyl)-2-[(9*H*-purin-6-yl)sulfanyl]ethan-1-one (**5**), C₁₄H₁₂N₄O₂S. Compounds (**2**), (**3**) and (**4**) are isomorphous and accordingly their molecular and supramolecular structures are similar. An analysis of the dihedral angles between the purine and exocyclic phenyl rings show that the molecules of (**1**) and (**5**) are essentially planar but that in the case of the three isomorphous compounds (**2**), (**3**) and (**4**), these rings are twisted by a dihedral angle of approximately 38°. With the exception of (**1**) all molecules are linked by weak C—H···O hydrogen bonds in their crystals. There is π – π stacking in all compounds. A Cambridge Structural Database search revealed the existence of 11 deposited compounds containing the 1-phenyl-2-sulfanylethanone scaffold; of these, only eight have a cyclic ring as substituent, the majority of these being heterocycles.

1. Chemical context

Purines, purine nucleosides and their analogs, are nitrogen-containing heterocycles ubiquitous in nature and present in biological systems like man, plants and marine organisms (Legraverend, 2008). These types of heterocycles take part of the core structure of guanine and adenine in nucleic acids (DNA and RNA) being involved in diverse *in vivo* catabolic and anabolic metabolic pathways.

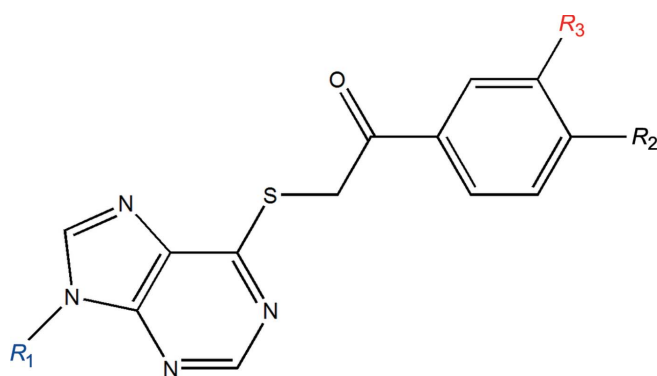
6-Mercaptopurine is a water insoluble purine analogue, which attracted attention due to its antitumor and immunosuppressive properties. The drug is used, among others, in the treatment of rheumatologic disorders, cancer and prevention of rejection of organ transplantation. The main problem associated with the pharmacological treatment with 6-mercaptopurine is the low bioavailability of the oral absorption and the short half-life in plasma. Strategies that have been adopted to circumvent those problems include the administration of 6-mercaptopurine analogues that act as prodrugs or by the chemical protection of the thiol group.

Chemically, the 6-mercaptopurine scaffold can also be modulated by an appropriate selection of the substituents that can be located at C-2, N-1, C-6, N-3, C-8, N-7 and N-9 posi-



tions, generating a variety of derivatives with potential biological applications (Legraverend & Grierson, 2006; Tunçbilek, *et al.*, 2009).

Within this framework, the goal of this project has been focused on the functionalization of 6-mercapto purine at positions 6 and 9. Here we describe the syntheses and characterization of five 6-mercaptapurine derivatives: 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(3-methoxyphenyl)ethan-1-one (**1**), 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-methoxyphenyl)ethan-1-one (**2**), 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-chlorophenyl)ethan-1-one (**3**), 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-bromophenyl)ethan-1-one (**4**) and 1-(3-methoxyphenyl)-2-[(9*H*-purin-6-yl)sulfanyl]ethan-1-one (**5**).



- | | | | |
|-----|-----------------------|----------------------|----------------------|
| (1) | $R_1 = \text{COCH}_3$ | $R_2 = \text{H}$ | $R_3 = \text{OCH}_3$ |
| (2) | $R_1 = \text{COCH}_3$ | $R_2 = \text{OCH}_3$ | $R_3 = \text{H}$ |
| (3) | $R_1 = \text{COCH}_3$ | $R_2 = \text{Cl}$ | $R_3 = \text{H}$ |
| (4) | $R_1 = \text{COCH}_3$ | $R_2 = \text{I}$ | $R_3 = \text{H}$ |
| (5) | $R_1 = \text{H}$ | $R_2 = \text{H}$ | $R_3 = \text{OCH}_3$ |

2. Structural commentary

Compounds (**1**)–(**5**) are shown in the scheme and their ellipsoid plots are shown in Figs. 1–5. Compounds (**1**) and (**5**) have similar *a* and *c* axes and (**2**), (**3**) and (**4**) are isostructural and isomorphous.

These compounds can be envisaged as two building blocks, a substituted phenylethanone grouping and a substituted 6-mercaptapurine moiety, bonded together by the mercapto ethanone residue. Since both purine and phenyl rings are essentially planar, the structural conformations of those compounds are conditioned by the $-\text{SCH}_2\text{CO}$ spacer (Fig. 6) which permits rotations around the following bonds: Pu–S6, S6–C61, C61–C62 and C62–Ph bonds. The sp^3 character of the central carbon atom may also direct the relative positions of the acetophenone residue out of the main plane constituted by the mercaptapurine, which is not the case of the present compounds. Selected geometric parameters for compounds (**1**)–(**5**) are given in Tables 1–5, respectively.

The Pu–S6 bond tends to be coplanar with the purine residue. In fact, the 6-mercaptapurine itself may appear in the thione form, *e.g.* 3,7-dihydropurine-6-thione, as a consequence of the high degree of electron delocalization within the 6-

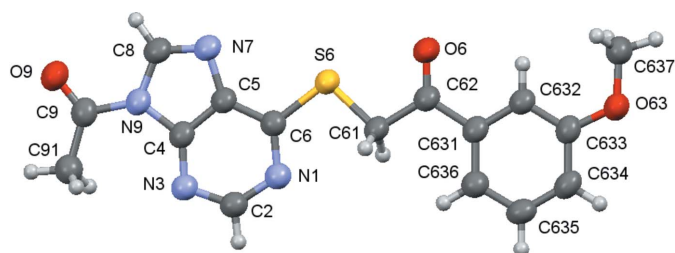


Figure 1
A view of the asymmetric unit of (**1**), with displacement ellipsoids are drawn at the 70% probability level.

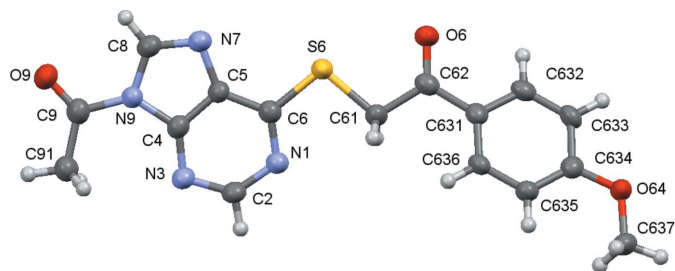


Figure 2
A view of the asymmetric unit of (**2**), with displacement ellipsoids are drawn at the 70% probability level.

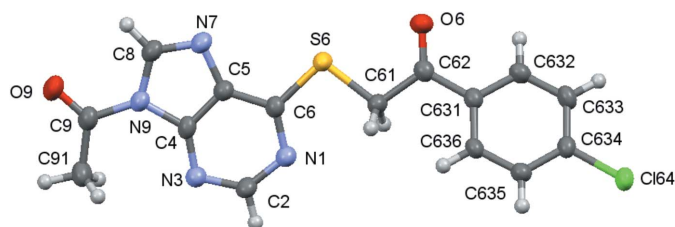


Figure 3
A view of the asymmetric unit of (**3**), with displacement ellipsoids are drawn at the 70% probability level.

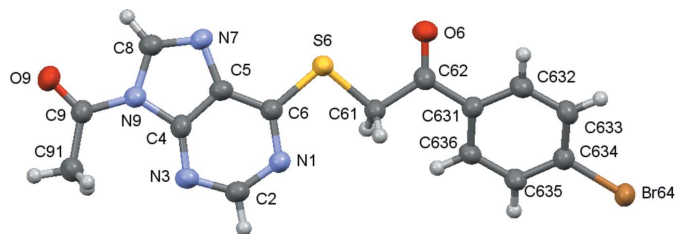


Figure 4
A view of the asymmetric unit of (**4**), with displacement ellipsoids are drawn at the 70% probability level.

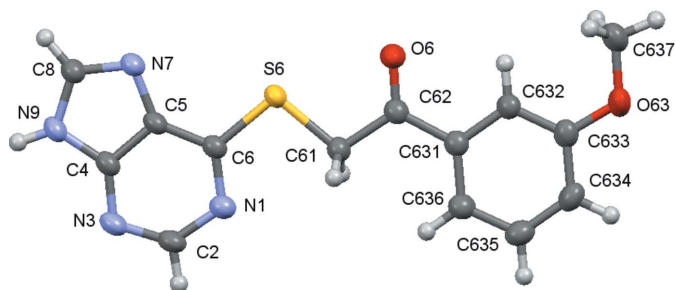


Figure 5
A view of the asymmetric unit of (**5**), with displacement ellipsoids are drawn at the 70% probability level.

Table 1
Selected geometric parameters (Å, °) for (1).

S6—C6	1.7438 (19)	C61—C62	1.520 (3)
S6—C61	1.8017 (18)	C62—C631	1.491 (3)
C6—S6—C61	100.76 (9)		
C6—S6—C61—C62	−178.05 (13)	S6—C61—C62—C631	−172.56 (14)
S6—C61—C62—O6	8.5 (2)		

Table 2
Selected geometric parameters (Å, °) for (2).

S6—C6	1.741 (3)	C61—C62	1.510 (4)
S6—C61	1.807 (3)	C62—C631	1.474 (3)
C6—S6—C61	100.88 (12)		
C6—S6—C61—C62	170.8 (2)	S6—C61—C62—C631	175.8 (2)
S6—C61—C62—O6	−7.7 (3)		

Table 3
Selected geometric parameters (Å, °) for (3).

S6—C6	1.7446 (18)	C61—C62	1.513 (2)
S6—C61	1.8038 (17)	C62—C631	1.493 (2)
C6—S6—C61	100.50 (8)		
C6—S6—C61—C62	177.77 (12)	S6—C61—C62—C631	177.32 (12)
S6—C61—C62—O6	−4.5 (2)		

Table 4
Selected geometric parameters (Å, °) for (4).

S6—C6	1.755 (3)	C61—C62	1.528 (4)
S6—C61	1.812 (3)	C62—C631	1.496 (4)
C6—S6—C61	100.33 (15)		
C6—S6—C61—C62	−177.8 (2)	S6—C61—C62—C631	−178.1 (2)
S6—C61—C62—O6	3.2 (4)		

Table 5
Selected geometric parameters (Å, °) for (5).

S6—C6	1.7477 (12)	C61—C62	1.5162 (16)
S6—C61	1.8109 (13)	C62—C631	1.4887 (17)
C6—S6—C61	100.77 (6)		
C6—S6—C61—C62	179.54 (8)	S6—C61—C62—C631	−175.65 (9)
S6—C61—C62—O6	5.56 (14)		

mercaptapurine environment. The tendency for the Pu—S6 bond to assume partial double-bond character is also seen in the present compounds, for which the corresponding Pu—S6 bond lengths lie between 1.741 (3) Å for (2) and 1.755 (3) Å for (4). In contrast, the S6—C61 bond lengths are longer, with values lying between 1.8017 (18) Å in (1) and 1.812 (3) Å in (4). This bond can also be bent with respect to the main mercaptapurine plane. The degree of bending may be evaluated by the distance of the C62 carbon atom from the mean plane consisting of the mercaptopyrimidine atoms. Those values [0.307 (3), 0.272 (4), 0.333 (2), 0.332 (4) and 0.164 (2)

Table 6
Selected dihedral angles (°).

θ_1 is the dihedral angle between the mean planes of the purine and phenyl rings and the phenyl ring. θ_2 is the dihedral angles between the mean planes of the purine ring and the plane defined by the S6/C61/C62/O6 atoms. θ_3 is the dihedral angle between the mean planes of the phenyl ring and the plane defined by the S6/C61/C62/O6 atoms.

Compound	θ_1°	θ_2°	θ_3°
(1)	2.95 (7)	8.45 (8)	5.87 (9)
(2)	38.89 (9)	17.05 (12)	22.72 (13)
(3)	38.67 (6)	14.23 (8)	27.82 (8)
(4)	37.11 (10)	13.58 (13)	26.82 (14)
(5)	4.74 (5)	5.30 (5)	3.42 (8)

The maximum deviations from the mean plane of the S—C—O bridging unit are for compounds (1)–(5) are 0.0457 (13), −0.041 (2), −0.023 (11), −0.017 (2) and 0.0302 (8) Å respectively. In all cases it is atom C42 which shows the maximum deviation.

for (1)–(5), respectively] show that the degree of bending is higher in (1)–(4) than in (5). As regards the ethanone group, the C61—C62 bond lengths lie in the range 1.510 (4) Å (2) to 1.528 (4) Å, (4) and are normal for a Csp^3 — Csp^3 bond while the C62—Ph bond lengths are shorter and lie in the range 1.474 (3) Å (2) to 1.496 (4) (4), suggesting that the electron density is delocalized from the phenyl ring.

The dihedral angles between the mean planes of the of the purine and phenyl ring, θ_1 , those between the mean plane of the purine ring and the plane defined by the S6—C61—C62—O6 atoms, θ_2 , and those between the mean planes of the phenyl ring and the plane defined by the S6—C61—C62—O6 atoms, θ_3 are given in Table 6. These values show that the molecules of (1) and (5) are essentially planar. However, in the case of the three isomorphous compounds (2), (3) and (4), the purine and exocyclic phenyl rings are both twisted in the opposite direction from the plane of the bridging unit, resulting in a dihedral angle of approximately 38°. This is due to the rotations and bending around the bonds connecting the bridging unit to the purine and exocyclic phenyl rings as discussed above. The dihedral angles θ_2 are higher than θ_3 ; the former are mainly due to the rotations around the S6—C61 bond while the latter are mainly the result of the bending of the C62—Ph bond.

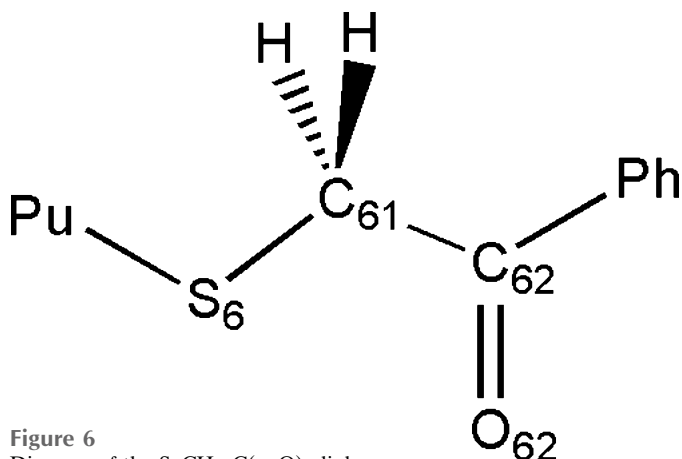


Figure 6
Diagram of the S—CH₂—C(=O)— linkage.

Table 7
Hydrogen-bond geometry (Å, °) for (2).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2···O64 ⁱ	0.95	2.48	3.375 (3)	157
C8—H8···O9 ⁱⁱ	0.95	2.37	3.319 (3)	178
C61—H61A···O6 ⁱⁱⁱ	0.99	2.33	3.269 (3)	159

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

Table 8
Hydrogen-bond geometry (Å, °) for (3).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8···O9 ⁱ	0.95	2.31	3.262 (2)	176
C61—H61A···O6 ⁱⁱ	0.99	2.40	3.354 (2)	162

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

Table 9
Hydrogen-bond geometry (Å, °) for (4).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C8—H8···O9 ⁱ	0.95	2.42	3.367 (4)	177
C61—H61B···O6 ⁱⁱ	0.99	2.45	3.396 (4)	160

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

Table 10
Hydrogen-bond geometry (Å, °) for (5).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N9—H9···N7 ⁱ	0.88	1.90	2.7715 (14)	171

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

3. Supramolecular features

There are no weak C—H···O or C—H···N contacts in (1). Hydrogen bonds for (2)–(5) are listed in Tables 7–10, respectively. Since (2), (3) and (4) are isomorphous, their supramolecular structures follow similar patterns. Accord-

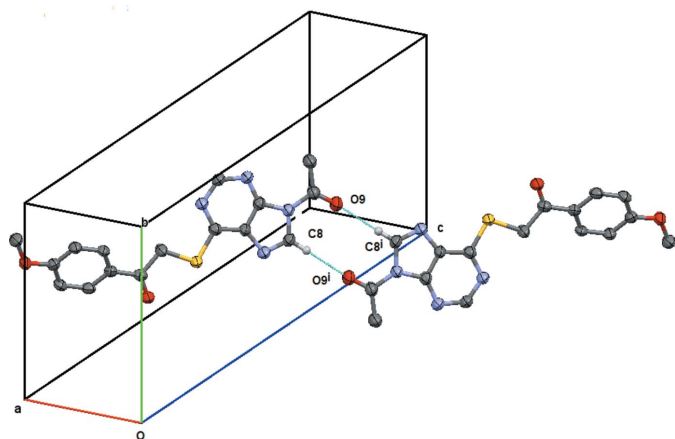


Figure 7
Compound (2): view of the C8—H8···O9 centrosymmetric $R_2^2(16)$ ring structure centred on $(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Symmetry code: (i) $-x - 1, -y + 1, -z + 1$. H atoms not involved in the hydrogen bonding are omitted.

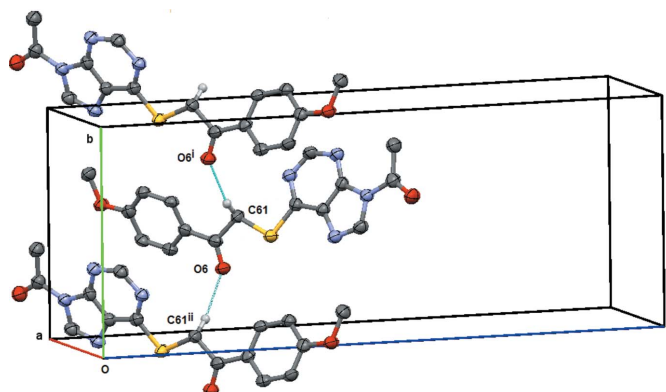


Figure 8
Compound (2): the simple C_4 chain formed by the C61—H61A···O6 weak hydrogen bond. This chain extends along the *b* axis and is generated by the twofold screw axis at $(\frac{1}{2}, y, \frac{1}{4})$. Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$. H atoms not involved in the hydrogen bonding are omitted.

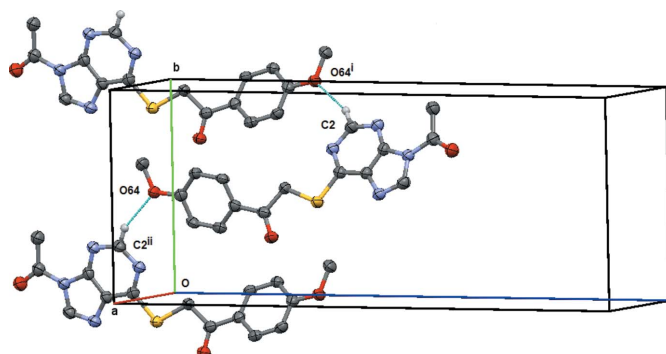


Figure 9
Compound (2): the simple C_{12} chain formed by the C2—H2···O64 weak hydrogen bond. This chain extends along the *b* axis and is generated by the twofold screw-axis at $(1, y, \frac{1}{4})$. Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$. H atoms not involved in the hydrogen bonding are omitted.

ingly, hydrogen-bonding diagrams are given for (2) only. Atom C8 acts as a donor to O9 ($-x - 1, -y + 1, -z + 1$), via H8 forming an $R_2^2(10)$ centrosymmetric dimer across the inversion centre at $(-1/2, 1/2, 1/2)$, Fig. 7. Atom C61 makes a hydrogen bond with O6 ($-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$), via H61A, forming a C_4 chain, which runs parallel to the *b* axis, Fig. 8, generated by the twofold screw axis at $(1/2, y, 1/4)$. In (2), there is a short contact between C6 and the 4-methoxy atom O64 ($-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$), forming a C_{12} chain, Fig. 9, which runs parallel to the *b* axis and is generated by the twofold screw axis at $(1, y, \frac{1}{4})$. In (5), the N9—H9···N9 ($x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$) hydrogen bond, Fig. 10, links the molecules into a C_4 chain which runs parallel to $[\bar{1}01]$ and which is generated by the *n*-glide plane at $(0, \frac{1}{4}, 0)$.

Since those compounds have three rings, the imidazole ring (with centroid Cg1), the pyrimidine ring (with centroid Cg2) and the benzyl ring (with centroid Cg3), it would be expected that π – π contacts were part of the supramolecular structure. Table 11 lists the possible π – π contacts for (1)–(5). As may be seen in the Table, the pyrimidine ring establishes π – π contacts with the benzyl ring for all compounds. In (1), two molecules centrosymmetrically related across the inversion centre at

Table 11

 Selected π - π contacts (\AA , $^\circ$).

$CgI(J)$ is plane $I(J)$; $Cg \cdots Cg$ is the distance between ring centroids; α is the dihedral angle between planes I and J ; CgI_{perp} is the perpendicular distance of $Cg(I)$ on ring J ; CgJ_{perp} is the perpendicular distance of $Cg(J)$ on ring I ; Slippage is the distance between $Cg(I)$ and the perpendicular projection of $Cg(J)$ on ring I . Plane 1 is through the imadazole ring, plane 2 the pyrimidine ring and plane 3 the exocyclic benzene ring.

Compound	CgI	CgJ	$Cg \cdots Cg$	α	CgI_{perp}	CgJ_{perp}	Slippage
(1)	$Cg1$	$Cg3(-x, 1-y, 1-z)$	3.6923 (14)	2.62 (12)	3.4547 (9)	-3.3985 (9)	
	$Cg2$	$Cg3(-x, 1-y, 1-z)$	3.6019 (12)	3.26 (11)	-3.3477 (9)	-3.4071 (9)	
(2)	$Cg1$	$Cg1(-x, 1-y, -z)$	3.8561 (16)	0.00 (15)	3.3156 (11)	3.3156 (11)	1.969
	$Cg2$	$Cg3(1-x, \frac{1}{2}+y, \frac{1}{2}-z)$	3.8270 (16)	0.80 (12)	-3.2463 (10)	-3.2391 (11)	
(3)	$Cg1$	$Cg1(-x, 1-y, -z)$	3.7799 (11)	0	3.2016 (7)	3.2016 (7)	2.009
	$Cg2$	$Cg3(1-x, \frac{1}{2}+y, \frac{1}{2}-z)$	4.0620 (10)	6.70 (8)	-3.4438 (7)	-3.1708 (7)	
(4)	$Cg1$	$Cg1(1-x, 1-y, 1-z)$	3.8319 (18)	0.04 (18)	3.1987 (13)	3.1987 (13)	2.110
	$Cg2$	$Cg3(1-x, \frac{1}{2}+y, \frac{1}{2}-z)$	4.1601 (18)	6.27 (15)	-3.4328 (12)	-3.1701 (13)	
(5)	$Cg1$	$Cg3(-x, 1-y, 1-z)$	3.6359 (8)	5.35 (7)	-3.4757 (5)	-3.4162 (5)	
	$Cg2$	$Cg3(-x, 1-y, 1-z)$	3.5204 (8)	4.43 (6)	-3.3669 (5)	-3.4160 (5)	

$(0, \frac{1}{2}, \frac{1}{2})$ are involved in π - π stacking in which the purine ring stacks above the exocyclic phenyl ring. In (2), (3) and (4), the π - π stacking is between imidazole rings while in (1) and (5), the contact is between an imidazole ring and a benzyl ring. In particular, in (1) and (5) two molecules centrosymmetrically related across the centre of symmetry at $(0, \frac{1}{2}, \frac{1}{2})$ are involved in π - π stacking in which the purine rings stack above the exocyclic phenyl ring, Table 11.

4. Database survey

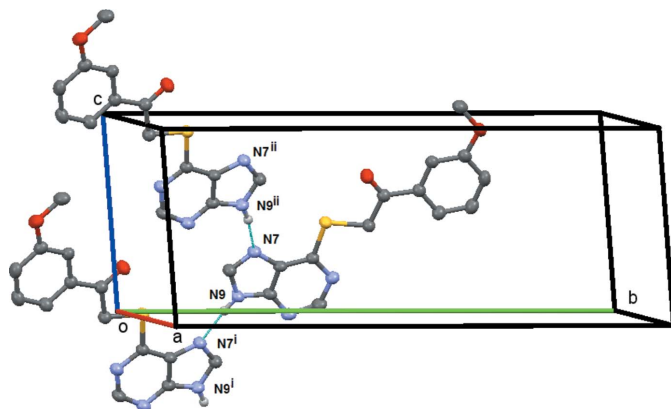
A search made in the Cambridge Structural Database (Groom & Allen, 2014) revealed the existence of 11 deposited compounds containing the 2-thio-1-phenylethanone scaffold (see supplementary Figure). Of those, only eight have a cyclic ring as substituent, the majority of these being heterocycles: MUCCUJ: 2-(1,3-benzoxazol-2-ylsulfanyl)-1-phenylethanone (Loghmani-Khouzani *et al.*, 2009a); NENFAO: 3-(benzoylmethylthio)-1,5-diphenyl-1H-1,2,4-triazole (Liu *et al.*, 2006); PUFGED: 2-(1,3-benzothiazol-2-ylsulfanyl)-1-phenylethan-

one (Loghmani-Khouzani *et al.*, 2009b); IKAXOI: 6-cyclohexylmethyl-5-ethyl-2-[(2-oxo-2-phenylethyl)sulfanyl]pyrimidin-4(3H)-one (Yan *et al.*, 2011); SILGAW: 2-(benzoylmethylsulfanyl)-6-benzyl-5-isopropylpyrimidin-4(3H)-one (Rao *et al.*, 2007); ETEWOP: 2-(benzoylmethylsulphanyl)-6-methoxy-1H-benzamide (Lynch & McLenaghan, 2004); XEBWEI: 2-(1,3-benzimidazol-2-ylsulfanyl)phenylethanone (Abdel-Aziz *et al.*, 2012); UGITUA: 2-[(4-methoxybenzyl)sulfanyl]-1-phenylethanone (Heravi *et al.*, 2009).

The R-S bond distances for these compounds are similar to those of the studied compounds and they assume a partial double-bond character with the exception of UGITUA where the S atom is bonded to a phenyl ring, suggesting a tendency for delocalization of the electron density through the sulfur atom when the ring has heteroatoms. The S-CH₂ bond distances vary between 1.80 and 1.81 \AA with exception of SILGAW (1.79 \AA) and ETEWOP (1.82 \AA). The supplementary figure also gives information about the distances of the -CH₂- carbon atom to the best plane made up of the atoms of the heterocycles (CH₂- distance). These values were computed in order to evaluate the degree of bending of the S-CH₂ bond with respect to the main plane of the substituted rings. There are two main groups of compounds, one in which the distance is shorter than 0.3 \AA and the other, which contains the CNH fragment in the heterocyclic ring, in which this distance is greater than 1.2 \AA . As noted above, the sp^3 character of the β -carbon atom of the ethanone fragment may also direct the relative positions of the acetophenone residue out of the main plane constituted by the substituted heteroaromatic ring. This is the case for SILGAW and IKAXOI. Thus, despite the small sample size, there is a wide range of adopted conformations.

5. Synthesis and crystallization

The 6-mercaptapurine derivatives (1)-(5) were obtained in moderate yields by a two-step synthetic strategy. Firstly, 6-mercaptapurine was alkylated using diverse monobromide acetophenone derivatives in DMF/potassium carbonate medium at room temperature (Lambertucci, *et al.* 2009). After


Figure 10

Compound (5): the simple C4 chain formed by the N9-H9...O64 weak hydrogen bond. This chain extends along the b axis and is generated by the n -glide plane at $(0, \frac{1}{4}, 0)$. Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z - \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{1}{2}$. H atoms not involved in the hydrogen bonding are omitted.

Table 12
Experimental details.

	(1)	(2)	(3)
Crystal data			
Chemical formula	C ₁₆ H ₁₄ N ₄ O ₃ S	C ₁₆ H ₁₄ N ₄ O ₃ S	C ₁₅ H ₁₁ ClN ₄ O ₂ S
<i>M_r</i>	342.37	342.37	346.79
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	100	100	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.6343 (5), 26.2356 (18), 8.1332 (5)	5.9920 (3), 9.9795 (5), 24.9907 (13)	5.9900 (4), 9.9169 (7), 24.3238 (17)
β (°)	112.725 (2)	95.977 (5)	96.072 (2)
<i>V</i> (Å ³)	1502.54 (17)	1486.25 (13)	1436.78 (17)
<i>Z</i>	4	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.24	0.24	0.43
Crystal size (mm)	0.17 × 0.07 × 0.01	0.05 × 0.04 × 0.01	0.13 × 0.06 × 0.01
Data collection			
Diffractometer	Rigaku AFC12 (Right)	Rigaku AFC12 (Right)	Rigaku AFC12 (Right)
Absorption correction	Multi-scan (<i>CrystalClear-SM Expert</i> ; Rigaku, 20112)	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2014)	Multi-scan (<i>CrystalClear-SM Expert</i> (Rigaku, 20112))
<i>T_{min}</i> , <i>T_{max}</i>	0, 1.000	0.439, 1.000	0.809, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	20144, 3450, 2817	15437, 2619, 1852	18353, 3291, 2677
<i>R_{int}</i>	0.089	0.106	0.050
(sin θ/λ) _{max} (Å ⁻¹)	0.649	0.595	0.651
Refinement			
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.053, 0.148, 1.05	0.048, 0.116, 1.02	0.035, 0.092, 1.02
No. of reflections	3450	2619	3291
No. of parameters	219	219	209
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.81, -0.51	0.30, -0.36	0.34, -0.22
	(4)	(5)	
Crystal data			
Chemical formula	C ₁₅ H ₁₁ BrN ₄ O ₂ S	C ₁₄ H ₁₂ N ₄ O ₂ S	
<i>M_r</i>	391.25	300.34	
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>	Monoclinic, <i>P</i> ₂ ₁ / <i>n</i>	
Temperature (K)	100	100	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.0705 (4), 10.0668 (7), 24.3492 (17)	7.6683 (5), 21.8004 (15), 8.4131 (5)	
β (°)	96.580 (2)	107.507 (2)	
<i>V</i> (Å ³)	1478.19 (18)	1341.29 (15)	
<i>Z</i>	4	4	
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	
μ (mm ⁻¹)	2.94	0.25	
Crystal size (mm)	0.15 × 0.10 × 0.02	0.17 × 0.12 × 0.07	
Data collection			
Diffractometer	Rigaku AFC12 (Right)	Rigaku AFC12 (Right)	
Absorption correction	Multi-scan (<i>CrystalClear-SM Expert</i> (Rigaku, 20112))	Multi-scan (<i>CrystalClear-SM Expert</i> ; Rigaku, 2012)	
<i>T_{min}</i> , <i>T_{max}</i>	0.658, 1.000	0.724, 1.000	
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	18171, 3346, 2944	17441, 3063, 2799	
<i>R_{int}</i>	0.064	0.060	
(sin θ/λ) _{max} (Å ⁻¹)	0.649	0.649	
Refinement			
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.056, 0.153, 1.06	0.033, 0.093, 1.03	
No. of reflections	3346	3063	
No. of parameters	209	191	
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	
Δρ _{max} , Δρ _{min} (e Å ⁻³)	2.91, -0.92	0.30, -0.37	

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2012), *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015a), *ShelXle* (Hübschle *et al.*, 2011), *SHELXL2014* (Sheldrick, 2015b), *OSCAIL* (McArdle *et al.*, 2004), *Mercury* (Macrae *et al.*, 2006), and *PLATON* (Spek, 2009).

thiol alkylation, the purine nucleus was acylated in position 9 with acetic anhydride in triethylamine and anhydrous DMF

for (1)–(4) under an argon atmosphere at room temperature (Masai, *et al.* 2002). All compounds were recrystallized from

dichloromethane solution: 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(3-methoxyphenyl)ethan-1-one (**1**): overall yield: 48%; m.p. 432–435 K; 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-methoxyphenyl)ethan-1-one (**2**): overall yield: 17%; m.p. 460–463 K; 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-chlorophenyl)ethan-1-one (**3**): overall yield: 26%; m.p. 453–457 K; 2-[(9-acetyl-9*H*-purin-6-yl)sulfanyl]-1-(4-bromophenyl)ethan-1-one (**4**): overall yield: 10%; m.p. 449–451 K; 1-(3-methoxyphenyl)-2-[(9*H*-purin-6-yl)sulfanyl]ethan-1-one (**5**): overall yield: 55%; m.p. 461–464 K.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 12. H atoms were treated as riding atoms with C–H(aromatic), 0.95 Å, with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$, C–H2(methylene), 0.99 Å, with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$, C–H(methyl) 0.98 Å with $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ and in (**5**) only, N–H, 0.88 Å, with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$. The positions of the methyl groups were checked on a final difference map as was that of the N–H hydrogen atom in (**5**). In (**4**), the high difference map peaks were associated with the Br atom.

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supporting information

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Crystal structures of five 6-mercaptapurine derivatives

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Computing details

Data collection: *CrystalClear-SM Expert* (Rigaku, 2012) for (1), (3), (4), (5); *CrysAlis PRO* (Agilent, 2014) for (2). Cell refinement: *CrystalClear-SM Expert* (Rigaku, 2012) for (1), (3), (4), (5); *CrysAlis PRO* (Agilent, 2014) for (2). Data reduction: *CrystalClear-SM Expert* (Rigaku, 2012) for (1), (3), (4), (5); *CrysAlis PRO* (Agilent, 2014) for (2). For all compounds, program(s) used to solve structure: *OSCAIL* (McArdle *et al.*, 2004) and *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *OSCAIL* (McArdle *et al.*, 2004), *ShelXle* (Hübschle *et al.*, 2011) and *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *OSCAIL* (McArdle *et al.*, 2004), *SHELXL2014* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

(1) 2-[(9-Acetyl-9H-purin-6-yl)sulfanyl]-1-(3-methoxyphenyl)ethan-1-one

Crystal data

$C_{16}H_{14}N_4O_3S$

$M_r = 342.37$

Monoclinic, $P2_1/n$

$a = 7.6343$ (5) Å

$b = 26.2356$ (18) Å

$c = 8.1332$ (5) Å

$\beta = 112.725$ (2)°

$V = 1502.54$ (17) Å³

$Z = 4$

$F(000) = 712$

$D_x = 1.513$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å

Cell parameters from 18327 reflections

$\theta = 2.7\text{--}27.5^\circ$

$\mu = 0.24$ mm⁻¹

$T = 100$ K

Plate, orange

$0.17 \times 0.07 \times 0.01$ mm

Data collection

Rigaku AFC12 (Right)
diffractometer

Radiation source: Rotating Anode

Detector resolution: 28.5714 pixels mm⁻¹

profile data from ω -scans

Absorption correction: multi-scan

(*CrystalClear-SM Expert*; Rigaku, 20112)

$T_{\min} = 0$, $T_{\max} = 1.000$

20144 measured reflections

3450 independent reflections

2817 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.089$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -9 \rightarrow 9$

$k = -33 \rightarrow 34$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.148$

$S = 1.05$

3450 reflections

219 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2 + 0.318P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$

$$\Delta\rho_{\max} = 0.81 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S6	0.32576 (7)	0.51901 (2)	0.60919 (6)	0.03400 (17)
O6	0.24518 (19)	0.61509 (5)	0.4576 (2)	0.0421 (4)
O9	0.8227 (2)	0.31676 (6)	1.1619 (2)	0.0427 (4)
O63	-0.20860 (19)	0.72411 (5)	-0.05304 (18)	0.0376 (3)
N1	0.2055 (2)	0.42325 (6)	0.4964 (2)	0.0331 (4)
N3	0.3481 (2)	0.34590 (6)	0.6538 (2)	0.0323 (4)
N7	0.6212 (2)	0.44997 (6)	0.9142 (2)	0.0340 (4)
N9	0.6216 (2)	0.36406 (6)	0.9348 (2)	0.0325 (4)
C2	0.2207 (3)	0.37227 (7)	0.5197 (3)	0.0342 (4)
H2	0.1291	0.3525	0.4292	0.041*
C4	0.4710 (3)	0.37649 (7)	0.7754 (3)	0.0309 (4)
C5	0.4740 (3)	0.42955 (7)	0.7676 (2)	0.0312 (4)
C6	0.3330 (3)	0.45263 (7)	0.6203 (2)	0.0308 (4)
C8	0.7025 (3)	0.41060 (7)	1.0084 (3)	0.0343 (4)
H8	0.8086	0.4132	1.1185	0.041*
C9	0.6911 (3)	0.31650 (7)	1.0206 (3)	0.0344 (4)
C61	0.1558 (3)	0.52851 (7)	0.3849 (2)	0.0321 (4)
H61A	0.1996	0.5115	0.2989	0.039*
H61B	0.0313	0.5139	0.3711	0.039*
C62	0.1376 (3)	0.58558 (7)	0.3504 (3)	0.0322 (4)
C91	0.5932 (3)	0.26954 (7)	0.9240 (3)	0.0396 (5)
H91A	0.6527	0.2394	0.9945	0.059*
H91B	0.6040	0.2678	0.8080	0.059*
H91C	0.4588	0.2707	0.9064	0.059*
C631	-0.0135 (2)	0.60328 (7)	0.1806 (2)	0.0312 (4)
C632	-0.0336 (3)	0.65606 (7)	0.1486 (2)	0.0317 (4)
H632	0.0474	0.6794	0.2332	0.038*
C633	-0.1734 (3)	0.67364 (7)	-0.0084 (3)	0.0328 (4)
C634	-0.2922 (3)	0.63923 (8)	-0.1321 (3)	0.0361 (4)
H634	-0.3883	0.6514	-0.2390	0.043*
C635	-0.2701 (3)	0.58745 (8)	-0.0994 (3)	0.0373 (4)
H635	-0.3502	0.5642	-0.1849	0.045*
C636	-0.1321 (3)	0.56914 (7)	0.0572 (3)	0.0352 (4)
H636	-0.1188	0.5335	0.0798	0.042*
C637	-0.0942 (3)	0.76081 (7)	0.0721 (3)	0.0396 (5)
H63A	0.0390	0.7563	0.0885	0.059*

H63B	-0.1070	0.7561	0.1864	0.059*
H63C	-0.1362	0.7952	0.0271	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S6	0.0278 (3)	0.0304 (3)	0.0354 (3)	0.00002 (17)	0.0030 (2)	-0.00035 (17)
O6	0.0327 (7)	0.0341 (7)	0.0442 (8)	-0.0027 (6)	-0.0019 (6)	0.0004 (6)
O9	0.0351 (8)	0.0417 (8)	0.0422 (8)	0.0012 (6)	0.0048 (7)	0.0043 (6)
O63	0.0322 (7)	0.0346 (7)	0.0376 (7)	0.0025 (5)	0.0042 (6)	0.0021 (5)
N1	0.0283 (8)	0.0332 (8)	0.0347 (8)	-0.0007 (6)	0.0088 (6)	-0.0002 (6)
N3	0.0280 (8)	0.0333 (8)	0.0337 (8)	-0.0013 (6)	0.0097 (7)	-0.0008 (6)
N7	0.0244 (8)	0.0361 (8)	0.0368 (9)	-0.0011 (6)	0.0066 (7)	-0.0020 (6)
N9	0.0241 (8)	0.0344 (8)	0.0358 (8)	0.0015 (6)	0.0080 (7)	0.0013 (6)
C2	0.0303 (9)	0.0347 (9)	0.0341 (10)	-0.0021 (7)	0.0087 (8)	-0.0023 (7)
C4	0.0236 (8)	0.0342 (9)	0.0336 (9)	0.0014 (7)	0.0096 (7)	0.0008 (7)
C5	0.0240 (8)	0.0324 (9)	0.0341 (9)	0.0000 (7)	0.0080 (7)	-0.0005 (7)
C6	0.0261 (9)	0.0309 (9)	0.0342 (9)	0.0002 (7)	0.0102 (8)	-0.0010 (7)
C8	0.0246 (8)	0.0378 (10)	0.0366 (10)	-0.0017 (7)	0.0076 (8)	-0.0022 (8)
C9	0.0280 (9)	0.0367 (10)	0.0389 (10)	0.0029 (7)	0.0133 (8)	0.0033 (8)
C61	0.0246 (9)	0.0324 (9)	0.0331 (10)	-0.0005 (7)	0.0041 (7)	0.0007 (7)
C62	0.0245 (8)	0.0342 (9)	0.0344 (9)	-0.0009 (7)	0.0077 (7)	-0.0003 (7)
C91	0.0345 (10)	0.0368 (10)	0.0442 (11)	0.0011 (8)	0.0115 (9)	0.0006 (8)
C631	0.0231 (8)	0.0362 (9)	0.0329 (9)	0.0000 (7)	0.0092 (7)	0.0010 (7)
C632	0.0249 (9)	0.0343 (9)	0.0326 (9)	-0.0007 (7)	0.0076 (7)	-0.0003 (7)
C633	0.0260 (9)	0.0360 (9)	0.0351 (10)	0.0032 (7)	0.0103 (8)	0.0028 (7)
C634	0.0266 (9)	0.0455 (11)	0.0318 (10)	0.0024 (8)	0.0065 (8)	0.0014 (8)
C635	0.0290 (9)	0.0423 (10)	0.0357 (10)	-0.0043 (8)	0.0072 (8)	-0.0058 (8)
C636	0.0301 (9)	0.0349 (9)	0.0374 (10)	-0.0014 (7)	0.0096 (8)	-0.0007 (7)
C637	0.0346 (10)	0.0351 (10)	0.0425 (11)	0.0010 (8)	0.0075 (9)	0.0011 (8)

Geometric parameters (Å, °)

S6—C6	1.7438 (19)	C61—C62	1.520 (3)
S6—C61	1.8017 (18)	C61—H61A	0.9900
O6—C62	1.217 (2)	C61—H61B	0.9900
O9—C9	1.199 (2)	C62—C631	1.491 (3)
O63—C633	1.372 (2)	C91—H91A	0.9800
O63—C637	1.428 (2)	C91—H91B	0.9800
N1—C6	1.341 (2)	C91—H91C	0.9800
N1—C2	1.350 (2)	C631—C636	1.388 (3)
N3—C4	1.336 (2)	C631—C632	1.407 (3)
N3—C2	1.340 (2)	C632—C633	1.389 (3)
N7—C8	1.293 (2)	C632—H632	0.9500
N7—C5	1.392 (2)	C633—C634	1.395 (3)
N9—C8	1.395 (2)	C634—C635	1.382 (3)
N9—C4	1.399 (2)	C634—H634	0.9500
N9—C9	1.428 (2)	C635—C636	1.388 (3)

C2—H2	0.9500	C635—H635	0.9500
C4—C5	1.394 (3)	C636—H636	0.9500
C5—C6	1.401 (2)	C637—H63A	0.9800
C8—H8	0.9500	C637—H63B	0.9800
C9—C91	1.496 (3)	C637—H63C	0.9800
C6—S6—C61	100.76 (9)	O6—C62—C61	120.45 (17)
C633—O63—C637	117.31 (15)	C631—C62—C61	117.42 (15)
C6—N1—C2	117.76 (16)	C9—C91—H91A	109.5
C4—N3—C2	111.95 (16)	C9—C91—H91B	109.5
C8—N7—C5	104.13 (16)	H91A—C91—H91B	109.5
C8—N9—C4	105.22 (15)	C9—C91—H91C	109.5
C8—N9—C9	122.41 (16)	H91A—C91—H91C	109.5
C4—N9—C9	132.36 (16)	H91B—C91—H91C	109.5
N3—C2—N1	128.47 (17)	C636—C631—C632	120.49 (17)
N3—C2—H2	115.8	C636—C631—C62	121.58 (17)
N1—C2—H2	115.8	C632—C631—C62	117.92 (16)
N3—C4—C5	125.80 (17)	C633—C632—C631	119.17 (17)
N3—C4—N9	129.53 (17)	C633—C632—H632	120.4
C5—C4—N9	104.66 (16)	C631—C632—H632	120.4
N7—C5—C4	111.55 (16)	O63—C633—C632	124.49 (17)
N7—C5—C6	131.72 (17)	O63—C633—C634	115.30 (16)
C4—C5—C6	116.73 (16)	C632—C633—C634	120.20 (17)
N1—C6—C5	119.27 (16)	C635—C634—C633	120.01 (18)
N1—C6—S6	122.38 (14)	C635—C634—H634	120.0
C5—C6—S6	118.31 (14)	C633—C634—H634	120.0
N7—C8—N9	114.43 (17)	C634—C635—C636	120.66 (18)
N7—C8—H8	122.8	C634—C635—H635	119.7
N9—C8—H8	122.8	C636—C635—H635	119.7
O9—C9—N9	118.60 (18)	C631—C636—C635	119.46 (18)
O9—C9—C91	124.84 (18)	C631—C636—H636	120.3
N9—C9—C91	116.55 (17)	C635—C636—H636	120.3
C62—C61—S6	107.55 (12)	O63—C637—H63A	109.5
C62—C61—H61A	110.2	O63—C637—H63B	109.5
S6—C61—H61A	110.2	H63A—C637—H63B	109.5
C62—C61—H61B	110.2	O63—C637—H63C	109.5
S6—C61—H61B	110.2	H63A—C637—H63C	109.5
H61A—C61—H61B	108.5	H63B—C637—H63C	109.5
O6—C62—C631	122.13 (17)		
C4—N3—C2—N1	0.3 (3)	C9—N9—C8—N7	-179.35 (18)
C6—N1—C2—N3	0.6 (3)	C8—N9—C9—O9	0.7 (3)
C2—N3—C4—C5	-1.2 (3)	C4—N9—C9—O9	-178.2 (2)
C2—N3—C4—N9	178.84 (19)	C8—N9—C9—C91	-178.60 (18)
C8—N9—C4—N3	179.7 (2)	C4—N9—C9—C91	2.5 (3)
C9—N9—C4—N3	-1.3 (4)	C6—S6—C61—C62	-178.05 (13)
C8—N9—C4—C5	-0.3 (2)	S6—C61—C62—O6	8.5 (2)
C9—N9—C4—C5	178.73 (19)	S6—C61—C62—C631	-172.56 (14)

C8—N7—C5—C4	−0.8 (2)	O6—C62—C631—C636	178.23 (19)
C8—N7—C5—C6	178.5 (2)	C61—C62—C631—C636	−0.7 (3)
N3—C4—C5—N7	−179.29 (18)	O6—C62—C631—C632	−2.1 (3)
N9—C4—C5—N7	0.7 (2)	C61—C62—C631—C632	179.03 (17)
N3—C4—C5—C6	1.3 (3)	C636—C631—C632—C633	−0.2 (3)
N9—C4—C5—C6	−178.75 (16)	C62—C631—C632—C633	−179.87 (17)
C2—N1—C6—C5	−0.5 (3)	C637—O63—C633—C632	−0.7 (3)
C2—N1—C6—S6	−178.35 (15)	C637—O63—C633—C634	178.19 (18)
N7—C5—C6—N1	−179.6 (2)	C631—C632—C633—O63	178.91 (17)
C4—C5—C6—N1	−0.3 (3)	C631—C632—C633—C634	0.1 (3)
N7—C5—C6—S6	−1.6 (3)	O63—C633—C634—C635	−179.39 (18)
C4—C5—C6—S6	177.61 (14)	C632—C633—C634—C635	−0.5 (3)
C61—S6—C6—N1	−12.10 (18)	C633—C634—C635—C636	0.9 (3)
C61—S6—C6—C5	170.02 (16)	C632—C631—C636—C635	0.6 (3)
C5—N7—C8—N9	0.6 (2)	C62—C631—C636—C635	−179.72 (18)
C4—N9—C8—N7	−0.2 (2)	C634—C635—C636—C631	−1.0 (3)

(2) 2-[(9-Acetyl-9H-purin-6-yl)sulfanyl]-1-(4-methoxyphenyl)ethan-1-one

*Crystal data*C₁₆H₁₄N₄O₃S $M_r = 342.37$ Monoclinic, $P2_1/c$ $a = 5.9920$ (3) Å $b = 9.9795$ (5) Å $c = 24.9907$ (13) Å $\beta = 95.977$ (5)° $V = 1486.25$ (13) Å³ $Z = 4$ $F(000) = 712$ $D_x = 1.530$ Mg m^{−3}Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5825 reflections

 $\theta = 2.2$ – 25.0 ° $\mu = 0.24$ mm^{−1} $T = 100$ K

Plate, colourless

 $0.05 \times 0.04 \times 0.01$ mm*Data collection*Rigaku AFC12 (Right)
diffractometerRadiation source: Rotating Anode, Rotating
Anode

Confocal mirrors, HF Varimax monochromator

Detector resolution: 28.5714 pixels mm^{−1}profile data from ω -scansAbsorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2014) $T_{\min} = 0.439$, $T_{\max} = 1.000$

15437 measured reflections

2619 independent reflections

1852 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.106$ $\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.2$ ° $h = -7$ → 6 $k = -11$ → 11 $l = -29$ → 29 *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.048$ $wR(F^2) = 0.116$ $S = 1.02$

2619 reflections

219 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.3956P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.30$ e Å^{−3} $\Delta\rho_{\min} = -0.36$ e Å^{−3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S6	0.34226 (12)	0.45424 (7)	0.33305 (3)	0.0300 (2)
O6	0.6113 (3)	0.30045 (19)	0.27249 (7)	0.0315 (5)
O9	-0.4124 (3)	0.6642 (2)	0.51385 (8)	0.0386 (6)
O64	1.2947 (3)	0.54050 (18)	0.12232 (7)	0.0331 (5)
N1	0.3919 (4)	0.7064 (2)	0.37258 (9)	0.0274 (6)
N3	0.1587 (4)	0.8075 (2)	0.43517 (9)	0.0282 (6)
N7	-0.0486 (4)	0.4737 (2)	0.41015 (9)	0.0295 (6)
N9	-0.1340 (4)	0.6524 (2)	0.45982 (8)	0.0268 (6)
C2	0.3246 (5)	0.8061 (3)	0.40336 (10)	0.0286 (7)
H2	0.4069	0.8873	0.4023	0.034*
C4	0.0500 (4)	0.6901 (3)	0.43323 (10)	0.0260 (7)
C5	0.0983 (4)	0.5794 (3)	0.40346 (10)	0.0251 (6)
C6	0.2774 (5)	0.5909 (3)	0.37190 (11)	0.0264 (7)
C8	-0.1807 (5)	0.5208 (3)	0.44369 (11)	0.0293 (7)
H8	-0.2989	0.4699	0.4561	0.035*
C9	-0.2672 (5)	0.7242 (3)	0.49399 (11)	0.0316 (7)
C61	0.5465 (5)	0.5280 (3)	0.29356 (11)	0.0296 (7)
H61A	0.4725	0.5938	0.2679	0.036*
H61B	0.6632	0.5752	0.3174	0.036*
C62	0.6521 (5)	0.4179 (3)	0.26328 (10)	0.0265 (7)
C91	-0.2175 (5)	0.8699 (3)	0.50110 (11)	0.0366 (8)
H91A	-0.2266	0.9134	0.4658	0.055*
H91B	-0.0662	0.8814	0.5195	0.055*
H91C	-0.3271	0.9106	0.5226	0.055*
C631	0.8133 (4)	0.4560 (3)	0.22523 (10)	0.0257 (6)
C632	0.9745 (5)	0.3617 (3)	0.21303 (10)	0.0279 (7)
H632	0.9736	0.2748	0.2285	0.033*
C633	1.1329 (5)	0.3927 (3)	0.17933 (10)	0.0278 (7)
H633	1.2425	0.3284	0.1719	0.033*
C634	1.1318 (5)	0.5197 (3)	0.15592 (11)	0.0279 (7)
C635	0.9733 (4)	0.6143 (3)	0.16630 (10)	0.0276 (7)
H635	0.9713	0.6998	0.1496	0.033*
C636	0.8169 (4)	0.5822 (3)	0.20161 (10)	0.0264 (7)
H636	0.7105	0.6477	0.2098	0.032*
C637	1.3246 (5)	0.6732 (3)	0.10294 (12)	0.0362 (8)
H63A	1.4617	0.6770	0.0848	0.054*
H63B	1.3370	0.7360	0.1332	0.054*
H63C	1.1955	0.6977	0.0775	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S6	0.0341 (4)	0.0194 (4)	0.0394 (4)	-0.0023 (3)	0.0176 (3)	-0.0022 (3)
O6	0.0380 (12)	0.0199 (12)	0.0388 (11)	-0.0023 (9)	0.0149 (10)	0.0002 (9)
O9	0.0413 (12)	0.0305 (13)	0.0479 (13)	-0.0035 (10)	0.0236 (11)	-0.0003 (10)
O64	0.0377 (12)	0.0206 (12)	0.0448 (12)	0.0004 (9)	0.0228 (10)	0.0014 (9)
N1	0.0290 (13)	0.0206 (14)	0.0340 (13)	-0.0009 (11)	0.0105 (11)	0.0005 (11)
N3	0.0297 (13)	0.0230 (14)	0.0333 (13)	-0.0040 (11)	0.0107 (11)	-0.0009 (10)
N7	0.0326 (14)	0.0206 (14)	0.0372 (13)	-0.0017 (11)	0.0128 (12)	0.0014 (11)
N9	0.0278 (13)	0.0205 (14)	0.0340 (13)	0.0006 (10)	0.0119 (11)	0.0012 (11)
C2	0.0292 (16)	0.0226 (17)	0.0352 (16)	-0.0051 (13)	0.0087 (14)	-0.0006 (13)
C4	0.0273 (16)	0.0251 (17)	0.0267 (15)	-0.0001 (13)	0.0081 (13)	0.0030 (12)
C5	0.0237 (14)	0.0217 (17)	0.0311 (15)	-0.0002 (12)	0.0091 (13)	0.0011 (12)
C6	0.0293 (15)	0.0223 (17)	0.0286 (15)	0.0013 (13)	0.0068 (13)	0.0007 (12)
C8	0.0279 (15)	0.0247 (18)	0.0366 (16)	-0.0026 (13)	0.0101 (14)	0.0031 (13)
C9	0.0320 (16)	0.0287 (18)	0.0358 (16)	0.0032 (14)	0.0116 (14)	0.0017 (13)
C61	0.0370 (17)	0.0208 (17)	0.0336 (16)	0.0006 (13)	0.0160 (14)	0.0024 (12)
C62	0.0305 (16)	0.0195 (17)	0.0296 (15)	0.0010 (13)	0.0030 (13)	-0.0020 (12)
C91	0.0425 (18)	0.0283 (18)	0.0421 (17)	-0.0003 (14)	0.0190 (16)	-0.0020 (14)
C631	0.0272 (15)	0.0210 (16)	0.0298 (15)	-0.0028 (12)	0.0066 (13)	-0.0049 (12)
C632	0.0360 (17)	0.0178 (16)	0.0303 (15)	-0.0002 (13)	0.0054 (14)	-0.0028 (12)
C633	0.0303 (15)	0.0197 (16)	0.0344 (15)	0.0056 (12)	0.0083 (14)	-0.0031 (13)
C634	0.0310 (16)	0.0236 (17)	0.0302 (15)	-0.0045 (13)	0.0090 (13)	-0.0033 (12)
C635	0.0316 (16)	0.0188 (16)	0.0338 (16)	-0.0006 (13)	0.0105 (14)	0.0011 (12)
C636	0.0271 (15)	0.0170 (16)	0.0362 (16)	0.0009 (12)	0.0091 (13)	-0.0033 (12)
C637	0.0448 (19)	0.0243 (17)	0.0430 (18)	-0.0049 (14)	0.0218 (16)	0.0008 (14)

Geometric parameters (Å, °)

S6—C6	1.741 (3)	C61—C62	1.510 (4)
S6—C61	1.807 (3)	C61—H61A	0.9900
O6—C62	1.224 (3)	C61—H61B	0.9900
O9—C9	1.206 (3)	C62—C631	1.474 (3)
O64—C634	1.368 (3)	C91—H91A	0.9800
O64—C637	1.428 (3)	C91—H91B	0.9800
N1—C6	1.340 (3)	C91—H91C	0.9800
N1—C2	1.345 (3)	C631—C636	1.393 (4)
N3—C2	1.336 (3)	C631—C632	1.404 (4)
N3—C4	1.339 (3)	C632—C633	1.368 (4)
N7—C8	1.299 (3)	C632—H632	0.9500
N7—C5	1.395 (3)	C633—C634	1.395 (4)
N9—C8	1.394 (3)	C633—H633	0.9500
N9—C4	1.396 (3)	C634—C635	1.383 (4)
N9—C9	1.422 (3)	C635—C636	1.389 (3)
C2—H2	0.9500	C635—H635	0.9500
C4—C5	1.379 (4)	C636—H636	0.9500
C5—C6	1.401 (4)	C637—H63A	0.9800

C8—H8	0.9500	C637—H63B	0.9800
C9—C91	1.491 (4)	C637—H63C	0.9800
C6—S6—C61	100.88 (12)	O6—C62—C61	120.0 (2)
C634—O64—C637	118.2 (2)	C631—C62—C61	118.2 (2)
C6—N1—C2	117.4 (2)	C9—C91—H91A	109.5
C2—N3—C4	111.0 (2)	C9—C91—H91B	109.5
C8—N7—C5	103.8 (2)	H91A—C91—H91B	109.5
C8—N9—C4	105.1 (2)	C9—C91—H91C	109.5
C8—N9—C9	122.7 (2)	H91A—C91—H91C	109.5
C4—N9—C9	132.1 (2)	H91B—C91—H91C	109.5
N3—C2—N1	129.3 (3)	C636—C631—C632	118.2 (2)
N3—C2—H2	115.3	C636—C631—C62	123.1 (2)
N1—C2—H2	115.3	C632—C631—C62	118.6 (2)
N3—C4—C5	126.3 (2)	C633—C632—C631	121.3 (3)
N3—C4—N9	128.6 (2)	C633—C632—H632	119.4
C5—C4—N9	105.2 (2)	C631—C632—H632	119.4
C4—C5—N7	111.7 (2)	C632—C633—C634	119.3 (2)
C4—C5—C6	117.0 (2)	C632—C633—H633	120.3
N7—C5—C6	131.2 (2)	C634—C633—H633	120.3
N1—C6—C5	119.0 (2)	O64—C634—C635	124.0 (2)
N1—C6—S6	122.46 (19)	O64—C634—C633	115.0 (2)
C5—C6—S6	118.6 (2)	C635—C634—C633	121.0 (2)
N7—C8—N9	114.2 (2)	C634—C635—C636	118.9 (3)
N7—C8—H8	122.9	C634—C635—H635	120.5
N9—C8—H8	122.9	C636—C635—H635	120.5
O9—C9—N9	118.1 (3)	C635—C636—C631	121.2 (2)
O9—C9—C91	125.4 (2)	C635—C636—H636	119.4
N9—C9—C91	116.5 (2)	C631—C636—H636	119.4
C62—C61—S6	108.70 (19)	O64—C637—H63A	109.5
C62—C61—H61A	109.9	O64—C637—H63B	109.5
S6—C61—H61A	109.9	H63A—C637—H63B	109.5
C62—C61—H61B	109.9	O64—C637—H63C	109.5
S6—C61—H61B	109.9	H63A—C637—H63C	109.5
H61A—C61—H61B	108.3	H63B—C637—H63C	109.5
O6—C62—C631	121.7 (2)		
C4—N3—C2—N1	-1.2 (4)	C9—N9—C8—N7	176.4 (2)
C6—N1—C2—N3	1.4 (4)	C8—N9—C9—O9	7.5 (4)
C2—N3—C4—C5	0.7 (4)	C4—N9—C9—O9	-176.6 (3)
C2—N3—C4—N9	-179.0 (3)	C8—N9—C9—C91	-171.1 (3)
C8—N9—C4—N3	179.8 (3)	C4—N9—C9—C91	4.8 (4)
C9—N9—C4—N3	3.4 (5)	C6—S6—C61—C62	170.8 (2)
C8—N9—C4—C5	0.1 (3)	S6—C61—C62—O6	-7.7 (3)
C9—N9—C4—C5	-176.3 (3)	S6—C61—C62—C631	175.8 (2)
N3—C4—C5—N7	-179.5 (3)	O6—C62—C631—C636	160.4 (3)
N9—C4—C5—N7	0.2 (3)	C61—C62—C631—C636	-23.1 (4)
N3—C4—C5—C6	-0.4 (4)	O6—C62—C631—C632	-21.1 (4)

N9—C4—C5—C6	179.3 (2)	C61—C62—C631—C632	155.4 (3)
C8—N7—C5—C4	-0.5 (3)	C636—C631—C632—C633	0.7 (4)
C8—N7—C5—C6	-179.4 (3)	C62—C631—C632—C633	-177.9 (3)
C2—N1—C6—C5	-0.9 (4)	C631—C632—C633—C634	-1.1 (4)
C2—N1—C6—S6	178.9 (2)	C637—O64—C634—C635	9.6 (4)
C4—C5—C6—N1	0.5 (4)	C637—O64—C634—C633	-171.3 (2)
N7—C5—C6—N1	179.4 (3)	C632—C633—C634—O64	-179.2 (2)
C4—C5—C6—S6	-179.3 (2)	C632—C633—C634—C635	0.0 (4)
N7—C5—C6—S6	-0.4 (4)	O64—C634—C635—C636	-179.4 (2)
C61—S6—C6—N1	-8.5 (3)	C633—C634—C635—C636	1.5 (4)
C61—S6—C6—C5	171.3 (2)	C634—C635—C636—C631	-1.9 (4)
C5—N7—C8—N9	0.6 (3)	C632—C631—C636—C635	0.9 (4)
C4—N9—C8—N7	-0.5 (3)	C62—C631—C636—C635	179.4 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O64 ⁱ	0.95	2.48	3.375 (3)	157
C8—H8...O9 ⁱⁱ	0.95	2.37	3.319 (3)	178
C61—H61A...O6 ⁱⁱⁱ	0.99	2.33	3.269 (3)	159

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

(3) 2-[(9-Acetyl-9H-purin-6-yl)sulfanyl]-1-(4-chlorophenyl)ethan-1-one*Crystal data*

C₁₅H₁₁ClN₄O₂S
M_r = 346.79
 Monoclinic, *P*2₁/*c*
a = 5.9900 (4) Å
b = 9.9169 (7) Å
c = 24.3238 (17) Å
 β = 96.072 (2)°
V = 1436.78 (17) Å³
Z = 4

F(000) = 712
D_x = 1.603 Mg m⁻³
 Mo *K* α radiation, λ = 0.71075 Å
 Cell parameters from 16488 reflections
 θ = 2.5–27.5°
 μ = 0.43 mm⁻¹
T = 100 K
 Plate, yellow
 0.13 × 0.06 × 0.01 mm

Data collection

Rigaku AFC12 (Right)
 diffractometer
 Radiation source: Rotating Anode
 Detector resolution: 28.5714 pixels mm⁻¹
 profile data from ω -scans
 Absorption correction: multi-scan
CrystalClear-SM Expert (Rigaku, 20112)
T_{min} = 0.809, *T_{max}* = 1.000

18353 measured reflections
 3291 independent reflections
 2677 reflections with *I* > 2 σ (*I*)
R_{int} = 0.050
 θ_{\max} = 27.5°, θ_{\min} = 2.7°
h = -7→7
k = -12→12
l = -31→31

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2 σ (*F*²)] = 0.035
wR(*F*²) = 0.092
S = 1.02

3291 reflections
 209 parameters
 0 restraints
 Hydrogen site location: inferred from
 neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.5802P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl64	1.32087 (7)	0.64277 (5)	0.10411 (2)	0.02661 (13)
S6	0.38690 (7)	0.47381 (4)	0.33773 (2)	0.02313 (12)
O6	0.6478 (2)	0.33342 (12)	0.26796 (5)	0.0267 (3)
O9	-0.4321 (2)	0.65965 (14)	0.51215 (6)	0.0325 (3)
N1	0.3921 (2)	0.73219 (15)	0.37483 (6)	0.0219 (3)
N3	0.1372 (2)	0.82388 (15)	0.43621 (6)	0.0227 (3)
N7	-0.0233 (2)	0.47859 (16)	0.41129 (6)	0.0242 (3)
N9	-0.1394 (2)	0.65498 (15)	0.46015 (6)	0.0223 (3)
C2	0.3079 (3)	0.82958 (18)	0.40503 (7)	0.0235 (4)
H2	0.3800	0.9148	0.4041	0.028*
C4	0.0447 (3)	0.70149 (19)	0.43464 (7)	0.0210 (3)
C5	0.1118 (3)	0.59112 (18)	0.40522 (7)	0.0209 (4)
C6	0.2939 (3)	0.61023 (18)	0.37446 (7)	0.0209 (4)
C8	-0.1682 (3)	0.52134 (18)	0.44384 (7)	0.0233 (4)
H8	-0.2836	0.4657	0.4554	0.028*
C9	-0.2805 (3)	0.72219 (19)	0.49567 (7)	0.0247 (4)
C61	0.5765 (3)	0.55799 (18)	0.29613 (7)	0.0231 (4)
H61A	0.4932	0.6245	0.2714	0.028*
H61B	0.6936	0.6065	0.3202	0.028*
C62	0.6837 (3)	0.45309 (18)	0.26215 (7)	0.0215 (4)
C91	-0.2263 (3)	0.8664 (2)	0.50911 (8)	0.0309 (4)
H91A	-0.2262	0.9181	0.4748	0.046*
H91B	-0.0778	0.8721	0.5302	0.046*
H91C	-0.3393	0.9036	0.5312	0.046*
C631	0.8399 (3)	0.50213 (18)	0.22261 (7)	0.0209 (4)
C632	1.0125 (3)	0.41672 (18)	0.20934 (7)	0.0235 (4)
H632	1.0258	0.3290	0.2250	0.028*
C633	1.1644 (3)	0.45870 (19)	0.17350 (7)	0.0238 (4)
H633	1.2840	0.4018	0.1653	0.029*
C634	1.1368 (3)	0.58612 (18)	0.15003 (7)	0.0215 (4)
C635	0.9650 (3)	0.67191 (18)	0.16161 (7)	0.0225 (4)
H635	0.9483	0.7580	0.1445	0.027*
C636	0.8181 (3)	0.63008 (18)	0.19851 (7)	0.0214 (4)
H636	0.7018	0.6887	0.2075	0.026*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl64	0.0226 (2)	0.0260 (2)	0.0333 (2)	0.00033 (17)	0.01226 (17)	-0.00087 (18)
S6	0.0242 (2)	0.0180 (2)	0.0288 (2)	-0.00324 (17)	0.01066 (17)	-0.00245 (17)
O6	0.0289 (7)	0.0185 (7)	0.0338 (7)	-0.0011 (5)	0.0085 (5)	0.0000 (5)
O9	0.0269 (7)	0.0309 (8)	0.0423 (8)	-0.0021 (6)	0.0161 (6)	0.0031 (6)
N1	0.0208 (7)	0.0204 (8)	0.0250 (8)	-0.0025 (6)	0.0051 (6)	-0.0009 (6)
N3	0.0225 (7)	0.0200 (8)	0.0264 (8)	-0.0019 (6)	0.0061 (6)	-0.0013 (6)
N7	0.0215 (7)	0.0220 (8)	0.0300 (8)	-0.0045 (6)	0.0064 (6)	0.0005 (6)
N9	0.0189 (7)	0.0221 (8)	0.0269 (8)	-0.0017 (6)	0.0065 (6)	0.0017 (6)
C2	0.0222 (8)	0.0211 (9)	0.0279 (9)	-0.0047 (7)	0.0062 (7)	-0.0018 (7)
C4	0.0167 (8)	0.0253 (9)	0.0215 (8)	0.0010 (7)	0.0043 (6)	0.0017 (7)
C5	0.0190 (8)	0.0202 (9)	0.0240 (9)	-0.0014 (7)	0.0039 (7)	0.0006 (7)
C6	0.0183 (8)	0.0220 (9)	0.0227 (8)	0.0001 (7)	0.0042 (6)	0.0003 (7)
C8	0.0190 (8)	0.0238 (9)	0.0277 (9)	-0.0027 (7)	0.0046 (7)	0.0032 (7)
C9	0.0204 (8)	0.0272 (10)	0.0273 (9)	0.0006 (7)	0.0063 (7)	0.0018 (7)
C61	0.0255 (9)	0.0184 (9)	0.0270 (9)	-0.0021 (7)	0.0103 (7)	-0.0003 (7)
C62	0.0199 (8)	0.0215 (9)	0.0232 (8)	0.0017 (7)	0.0025 (6)	-0.0008 (7)
C91	0.0274 (9)	0.0307 (11)	0.0366 (11)	-0.0025 (8)	0.0134 (8)	-0.0072 (8)
C631	0.0193 (8)	0.0202 (9)	0.0235 (9)	-0.0001 (7)	0.0045 (7)	-0.0025 (7)
C632	0.0252 (9)	0.0182 (9)	0.0275 (9)	0.0031 (7)	0.0048 (7)	0.0009 (7)
C633	0.0202 (8)	0.0248 (10)	0.0270 (9)	0.0051 (7)	0.0050 (7)	-0.0022 (7)
C634	0.0187 (8)	0.0225 (9)	0.0239 (9)	-0.0017 (7)	0.0058 (7)	-0.0032 (7)
C635	0.0232 (8)	0.0173 (9)	0.0279 (9)	0.0008 (7)	0.0062 (7)	-0.0003 (7)
C636	0.0200 (8)	0.0181 (9)	0.0270 (9)	0.0018 (7)	0.0063 (7)	-0.0030 (7)

Geometric parameters (\AA , $^\circ$)

Cl64—C634	1.7433 (17)	C9—C91	1.495 (3)
S6—C6	1.7446 (18)	C61—C62	1.513 (2)
S6—C61	1.8038 (17)	C61—H61A	0.9900
O6—C62	1.217 (2)	C61—H61B	0.9900
O9—C9	1.203 (2)	C62—C631	1.493 (2)
N1—C2	1.344 (2)	C91—H91A	0.9800
N1—C6	1.344 (2)	C91—H91B	0.9800
N3—C4	1.333 (2)	C91—H91C	0.9800
N3—C2	1.337 (2)	C631—C636	1.398 (2)
N7—C8	1.306 (2)	C631—C632	1.400 (2)
N7—C5	1.395 (2)	C632—C633	1.389 (2)
N9—C8	1.389 (2)	C632—H632	0.9500
N9—C4	1.400 (2)	C633—C634	1.389 (3)
N9—C9	1.435 (2)	C633—H633	0.9500
C2—H2	0.9500	C634—C635	1.387 (2)
C4—C5	1.390 (2)	C635—C636	1.385 (2)
C5—C6	1.400 (2)	C635—H635	0.9500
C8—H8	0.9500	C636—H636	0.9500

C6—S6—C61	100.50 (8)	S6—C61—H61B	110.0
C2—N1—C6	117.46 (15)	H61A—C61—H61B	108.4
C4—N3—C2	111.27 (15)	O6—C62—C631	121.52 (16)
C8—N7—C5	103.57 (15)	O6—C62—C61	121.13 (16)
C8—N9—C4	105.53 (14)	C631—C62—C61	117.33 (15)
C8—N9—C9	123.49 (15)	C9—C91—H91A	109.5
C4—N9—C9	130.97 (15)	C9—C91—H91B	109.5
N3—C2—N1	129.31 (16)	H91A—C91—H91B	109.5
N3—C2—H2	115.3	C9—C91—H91C	109.5
N1—C2—H2	115.3	H91A—C91—H91C	109.5
N3—C4—C5	126.14 (15)	H91B—C91—H91C	109.5
N3—C4—N9	129.20 (16)	C636—C631—C632	119.40 (16)
C5—C4—N9	104.65 (15)	C636—C631—C62	121.92 (15)
C4—C5—N7	111.89 (15)	C632—C631—C62	118.68 (16)
C4—C5—C6	116.91 (16)	C633—C632—C631	120.80 (17)
N7—C5—C6	131.18 (16)	C633—C632—H632	119.6
N1—C6—C5	118.90 (16)	C631—C632—H632	119.6
N1—C6—S6	122.55 (12)	C632—C633—C634	118.25 (16)
C5—C6—S6	118.54 (13)	C632—C633—H633	120.9
N7—C8—N9	114.35 (15)	C634—C633—H633	120.9
N7—C8—H8	122.8	C635—C634—C633	122.19 (16)
N9—C8—H8	122.8	C635—C634—Cl64	117.76 (14)
O9—C9—N9	118.34 (17)	C633—C634—Cl64	120.05 (13)
O9—C9—C91	125.05 (17)	C636—C635—C634	118.94 (16)
N9—C9—C91	116.61 (15)	C636—C635—H635	120.5
C62—C61—S6	108.47 (12)	C634—C635—H635	120.5
C62—C61—H61A	110.0	C635—C636—C631	120.38 (16)
S6—C61—H61A	110.0	C635—C636—H636	119.8
C62—C61—H61B	110.0	C631—C636—H636	119.8
C4—N3—C2—N1	-0.7 (3)	C4—N9—C8—N7	0.2 (2)
C6—N1—C2—N3	0.7 (3)	C9—N9—C8—N7	179.77 (16)
C2—N3—C4—C5	0.2 (3)	C8—N9—C9—O9	-0.1 (3)
C2—N3—C4—N9	-178.24 (17)	C4—N9—C9—O9	179.26 (18)
C8—N9—C4—N3	178.49 (18)	C8—N9—C9—C91	-179.93 (17)
C9—N9—C4—N3	-1.0 (3)	C4—N9—C9—C91	-0.5 (3)
C8—N9—C4—C5	-0.24 (18)	C6—S6—C61—C62	177.77 (12)
C9—N9—C4—C5	-179.73 (17)	S6—C61—C62—O6	-4.5 (2)
N3—C4—C5—N7	-178.60 (16)	S6—C61—C62—C631	177.32 (12)
N9—C4—C5—N7	0.2 (2)	O6—C62—C631—C636	153.51 (18)
N3—C4—C5—C6	0.2 (3)	C61—C62—C631—C636	-28.3 (2)
N9—C4—C5—C6	178.95 (15)	O6—C62—C631—C632	-26.3 (3)
C8—N7—C5—C4	-0.1 (2)	C61—C62—C631—C632	151.92 (17)
C8—N7—C5—C6	-178.58 (19)	C636—C631—C632—C633	1.3 (3)
C2—N1—C6—C5	-0.1 (2)	C62—C631—C632—C633	-178.87 (16)
C2—N1—C6—S6	-179.32 (13)	C631—C632—C633—C634	-1.7 (3)
C4—C5—C6—N1	-0.2 (2)	C632—C633—C634—C635	0.5 (3)
N7—C5—C6—N1	178.25 (17)	C632—C633—C634—Cl64	-179.20 (13)

C4—C5—C6—S6	179.00 (13)	C633—C634—C635—C636	1.1 (3)
N7—C5—C6—S6	-2.5 (3)	Cl64—C634—C635—C636	-179.18 (13)
C61—S6—C6—N1	-11.73 (17)	C634—C635—C636—C631	-1.5 (3)
C61—S6—C6—C5	169.08 (14)	C632—C631—C636—C635	0.3 (3)
C5—N7—C8—N9	-0.1 (2)	C62—C631—C636—C635	-179.47 (16)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C8—H8 \cdots O9 ⁱ	0.95	2.31	3.262 (2)	176
C61—H61A \cdots O6 ⁱⁱ	0.99	2.40	3.354 (2)	162

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

(4) 2-[(9-Acetyl-9H-purin-6-yl)sulfanyl]-1-(4-bromophenyl)ethan-1-one*Crystal data*

$\text{C}_{15}\text{H}_{11}\text{BrN}_4\text{O}_2\text{S}$
 $M_r = 391.25$
 Monoclinic, $P2_1/c$
 $a = 6.0705$ (4) \AA
 $b = 10.0668$ (7) \AA
 $c = 24.3492$ (17) \AA
 $\beta = 96.580$ (2) $^\circ$
 $V = 1478.19$ (18) \AA^3
 $Z = 4$

$F(000) = 784$
 $D_x = 1.758$ Mg m^{-3}
 Mo $K\alpha$ radiation, $\lambda = 0.71075$ \AA
 Cell parameters from 18109 reflections
 $\theta = 2.5$ – 27.5 $^\circ$
 $\mu = 2.94$ mm^{-1}
 $T = 100$ K
 Plate, colourless
 $0.15 \times 0.10 \times 0.02$ mm

Data collection

Rigaku AFC12 (Right)
 diffractometer
 Radiation source: Rotating Anode
 Detector resolution: 28.5714 pixels mm^{-1}
 profile data from ω -scans
 Absorption correction: multi-scan
CrystalClear-SM Expert (Rigaku, 20112)
 $T_{\min} = 0.658$, $T_{\max} = 1.000$

18171 measured reflections
 3346 independent reflections
 2944 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\max} = 27.5$ $^\circ$, $\theta_{\min} = 2.6$ $^\circ$
 $h = -7 \rightarrow 7$
 $k = -12 \rightarrow 13$
 $l = -31 \rightarrow 31$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.153$
 $S = 1.06$
 3346 reflections
 209 parameters
 0 restraints

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1178P)^2 + 0.358P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.91$ e \AA^{-3}
 $\Delta\rho_{\min} = -0.92$ e \AA^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br64	1.32442 (5)	0.33869 (3)	0.10086 (2)	0.02971 (16)
S6	0.38570 (14)	0.51673 (7)	0.33803 (3)	0.0278 (2)
O6	0.6441 (5)	0.6537 (2)	0.26801 (11)	0.0318 (5)
O9	-0.4299 (5)	0.3392 (2)	0.51161 (11)	0.0357 (6)
N1	0.3870 (5)	0.2608 (3)	0.37506 (10)	0.0267 (5)
N3	0.1320 (5)	0.1721 (2)	0.43630 (12)	0.0279 (6)
N7	-0.0199 (5)	0.5157 (3)	0.41162 (11)	0.0274 (5)
N9	-0.1388 (5)	0.3411 (2)	0.46032 (12)	0.0263 (6)
C2	0.3003 (6)	0.1653 (3)	0.40499 (14)	0.0290 (7)
H2	0.3683	0.0806	0.4038	0.035*
C4	0.0420 (5)	0.2942 (3)	0.43479 (12)	0.0260 (6)
C5	0.1121 (5)	0.4027 (3)	0.40513 (12)	0.0262 (6)
C6	0.2904 (5)	0.3823 (3)	0.37469 (12)	0.0255 (6)
C8	-0.1649 (5)	0.4742 (3)	0.44429 (12)	0.0274 (6)
H8	-0.2771	0.5298	0.4559	0.033*
C9	-0.2823 (5)	0.2762 (3)	0.49460 (13)	0.0279 (6)
C61	0.5714 (5)	0.4314 (3)	0.29665 (13)	0.0278 (6)
H61A	0.6861	0.3827	0.3209	0.033*
H61B	0.4876	0.3666	0.2718	0.033*
C62	0.6802 (5)	0.5351 (3)	0.26272 (12)	0.0267 (6)
C91	-0.2352 (6)	0.1307 (4)	0.50629 (16)	0.0346 (7)
H91A	-0.2341	0.0827	0.4713	0.052*
H91B	-0.3506	0.0937	0.5268	0.052*
H91C	-0.0904	0.1214	0.5283	0.052*
C631	0.8358 (5)	0.4855 (3)	0.22393 (12)	0.0248 (6)
C632	1.0055 (6)	0.5701 (3)	0.20986 (13)	0.0292 (6)
H632	1.0178	0.6572	0.2250	0.035*
C633	1.1556 (5)	0.5285 (3)	0.17420 (13)	0.0282 (6)
H633	1.2725	0.5850	0.1657	0.034*
C634	1.1296 (5)	0.4012 (3)	0.15118 (12)	0.0262 (6)
C635	0.9596 (6)	0.3157 (3)	0.16372 (14)	0.0291 (6)
H635	0.9435	0.2301	0.1473	0.035*
C636	0.8144 (6)	0.3585 (3)	0.20067 (14)	0.0273 (6)
H636	0.7005	0.3009	0.2100	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br64	0.0279 (2)	0.0250 (2)	0.0387 (2)	0.00019 (11)	0.01488 (15)	0.00074 (10)
S6	0.0299 (4)	0.0199 (4)	0.0361 (4)	0.0021 (3)	0.0142 (3)	0.0016 (3)
O6	0.0370 (13)	0.0205 (12)	0.0399 (12)	0.0015 (9)	0.0127 (10)	-0.0010 (8)
O9	0.0334 (14)	0.0301 (14)	0.0469 (14)	0.0016 (9)	0.0193 (11)	-0.0011 (9)
N1	0.0255 (13)	0.0225 (13)	0.0335 (12)	0.0028 (10)	0.0101 (10)	0.0010 (10)
N3	0.0316 (15)	0.0206 (13)	0.0328 (13)	0.0045 (10)	0.0095 (11)	0.0032 (9)
N7	0.0258 (13)	0.0214 (13)	0.0366 (13)	0.0036 (10)	0.0104 (10)	-0.0008 (10)

N9	0.0266 (14)	0.0206 (14)	0.0332 (13)	0.0012 (9)	0.0096 (11)	-0.0011 (9)
C2	0.0296 (16)	0.0222 (16)	0.0365 (16)	0.0043 (11)	0.0087 (13)	0.0015 (11)
C4	0.0260 (15)	0.0258 (16)	0.0277 (13)	-0.0002 (12)	0.0091 (11)	-0.0006 (12)
C5	0.0267 (16)	0.0202 (15)	0.0325 (14)	0.0035 (11)	0.0065 (11)	0.0008 (11)
C6	0.0249 (15)	0.0209 (14)	0.0316 (14)	0.0006 (11)	0.0070 (11)	0.0007 (12)
C8	0.0284 (16)	0.0214 (15)	0.0332 (14)	0.0025 (11)	0.0070 (11)	-0.0002 (11)
C9	0.0255 (15)	0.0255 (16)	0.0342 (14)	-0.0002 (12)	0.0097 (11)	-0.0009 (12)
C61	0.0298 (16)	0.0202 (15)	0.0358 (14)	0.0003 (11)	0.0143 (12)	-0.0001 (12)
C62	0.0269 (16)	0.0230 (15)	0.0312 (14)	-0.0026 (11)	0.0081 (11)	-0.0012 (11)
C91	0.0343 (18)	0.0275 (16)	0.0448 (18)	0.0033 (14)	0.0162 (14)	0.0072 (14)
C631	0.0251 (15)	0.0218 (15)	0.0287 (13)	0.0013 (11)	0.0079 (11)	-0.0003 (11)
C632	0.0317 (16)	0.0207 (15)	0.0364 (15)	-0.0020 (12)	0.0098 (12)	-0.0007 (12)
C633	0.0272 (16)	0.0246 (16)	0.0339 (14)	-0.0036 (12)	0.0086 (11)	0.0017 (12)
C634	0.0246 (15)	0.0232 (15)	0.0321 (14)	0.0001 (11)	0.0085 (11)	0.0015 (11)
C635	0.0318 (17)	0.0199 (14)	0.0376 (15)	-0.0025 (12)	0.0127 (13)	-0.0016 (12)
C636	0.0288 (16)	0.0187 (14)	0.0360 (15)	-0.0017 (11)	0.0098 (13)	0.0011 (11)

Geometric parameters (Å, °)

Br64—C634	1.905 (3)	C9—C91	1.513 (5)
S6—C6	1.755 (3)	C61—C62	1.528 (4)
S6—C61	1.812 (3)	C61—H61A	0.9900
O6—C62	1.224 (4)	C61—H61B	0.9900
O9—C9	1.209 (4)	C62—C631	1.496 (4)
N1—C2	1.349 (4)	C91—H91A	0.9800
N1—C6	1.356 (4)	C91—H91B	0.9800
N3—C4	1.344 (4)	C91—H91C	0.9800
N3—C2	1.345 (5)	C631—C636	1.398 (4)
N7—C8	1.320 (4)	C631—C632	1.409 (5)
N7—C5	1.411 (4)	C632—C633	1.393 (5)
N9—C8	1.399 (4)	C632—H632	0.9500
N9—C4	1.404 (4)	C633—C634	1.400 (4)
N9—C9	1.431 (4)	C633—H633	0.9500
C2—H2	0.9500	C634—C635	1.404 (4)
C4—C5	1.402 (4)	C635—C636	1.398 (5)
C5—C6	1.395 (4)	C635—H635	0.9500
C8—H8	0.9500	C636—H636	0.9500
C6—S6—C61	100.33 (15)	S6—C61—H61B	110.1
C2—N1—C6	116.8 (3)	H61A—C61—H61B	108.4
C4—N3—C2	111.3 (3)	O6—C62—C631	121.7 (3)
C8—N7—C5	103.8 (3)	O6—C62—C61	121.1 (3)
C8—N9—C4	105.5 (3)	C631—C62—C61	117.2 (3)
C8—N9—C9	122.9 (3)	C9—C91—H91A	109.5
C4—N9—C9	131.6 (3)	C9—C91—H91B	109.5
N3—C2—N1	129.7 (3)	H91A—C91—H91B	109.5
N3—C2—H2	115.1	C9—C91—H91C	109.5
N1—C2—H2	115.1	H91A—C91—H91C	109.5

N3—C4—C5	125.4 (3)	H91B—C91—H91C	109.5
N3—C4—N9	129.2 (3)	C636—C631—C632	119.4 (3)
C5—C4—N9	105.4 (3)	C636—C631—C62	121.6 (3)
C6—C5—C4	117.3 (3)	C632—C631—C62	118.9 (3)
C6—C5—N7	131.5 (3)	C633—C632—C631	121.2 (3)
C4—C5—N7	111.1 (3)	C633—C632—H632	119.4
N1—C6—C5	119.4 (3)	C631—C632—H632	119.4
N1—C6—S6	122.1 (2)	C632—C633—C634	118.2 (3)
C5—C6—S6	118.5 (2)	C632—C633—H633	120.9
N7—C8—N9	114.2 (3)	C634—C633—H633	120.9
N7—C8—H8	122.9	C633—C634—C635	121.7 (3)
N9—C8—H8	122.9	C633—C634—Br64	120.7 (2)
O9—C9—N9	119.0 (3)	C635—C634—Br64	117.6 (2)
O9—C9—C91	125.1 (3)	C636—C635—C634	119.0 (3)
N9—C9—C91	115.9 (3)	C636—C635—H635	120.5
C62—C61—S6	108.2 (2)	C634—C635—H635	120.5
C62—C61—H61A	110.1	C635—C636—C631	120.4 (3)
S6—C61—H61A	110.1	C635—C636—H636	119.8
C62—C61—H61B	110.1	C631—C636—H636	119.8
C4—N3—C2—N1	1.4 (5)	C4—N9—C8—N7	-0.1 (4)
C6—N1—C2—N3	-1.6 (5)	C9—N9—C8—N7	-178.5 (3)
C2—N3—C4—C5	-0.5 (5)	C8—N9—C9—O9	-1.6 (5)
C2—N3—C4—N9	178.1 (3)	C4—N9—C9—O9	-179.6 (3)
C8—N9—C4—N3	-178.8 (3)	C8—N9—C9—C91	177.9 (3)
C9—N9—C4—N3	-0.6 (6)	C4—N9—C9—C91	0.0 (5)
C8—N9—C4—C5	0.0 (3)	C6—S6—C61—C62	-177.8 (2)
C9—N9—C4—C5	178.2 (3)	S6—C61—C62—O6	3.2 (4)
N3—C4—C5—C6	-0.1 (5)	S6—C61—C62—C631	-178.1 (2)
N9—C4—C5—C6	-179.0 (3)	O6—C62—C631—C636	-153.8 (3)
N3—C4—C5—N7	179.0 (3)	C61—C62—C631—C636	27.6 (4)
N9—C4—C5—N7	0.1 (3)	O6—C62—C631—C632	25.1 (4)
C8—N7—C5—C6	178.7 (3)	C61—C62—C631—C632	-153.6 (3)
C8—N7—C5—C4	-0.2 (3)	C636—C631—C632—C633	-1.5 (5)
C2—N1—C6—C5	0.8 (4)	C62—C631—C632—C633	179.6 (3)
C2—N1—C6—S6	179.6 (2)	C631—C632—C633—C634	1.9 (5)
C4—C5—C6—N1	-0.1 (4)	C632—C633—C634—C635	-0.8 (5)
N7—C5—C6—N1	-179.0 (3)	C632—C633—C634—Br64	178.7 (2)
C4—C5—C6—S6	-178.9 (2)	C633—C634—C635—C636	-0.8 (5)
N7—C5—C6—S6	2.2 (5)	Br64—C634—C635—C636	179.8 (2)
C61—S6—C6—N1	12.0 (3)	C634—C635—C636—C631	1.2 (5)
C61—S6—C6—C5	-169.3 (3)	C632—C631—C636—C635	-0.1 (5)
C5—N7—C8—N9	0.2 (4)	C62—C631—C636—C635	178.8 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8 \cdots O9 ⁱ	0.95	2.42	3.367 (4)	177

C61—H61B···O6ⁱⁱ 0.99 2.45 3.396 (4) 160

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

(5) 1-(3-Methoxyphenyl)-2-[(9*H*-purin-6-yl)sulfanyl]ethan-1-one

Crystal data

C ₁₄ H ₁₂ N ₄ O ₂ S	$F(000) = 624$
$M_r = 300.34$	$D_x = 1.487 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$
$a = 7.6683 (5) \text{ \AA}$	Cell parameters from 16870 reflections
$b = 21.8004 (15) \text{ \AA}$	$\theta = 2.5\text{--}27.5^\circ$
$c = 8.4131 (5) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$\beta = 107.507 (2)^\circ$	$T = 100 \text{ K}$
$V = 1341.29 (15) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.17 \times 0.12 \times 0.07 \text{ mm}$

Data collection

Rigaku AFC12 (Right) diffractometer	17441 measured reflections
Radiation source: Rotating Anode	3063 independent reflections
Detector resolution: $28.5714 \text{ pixels mm}^{-1}$	2799 reflections with $I > 2\sigma(I)$
profile data from ω -scans	$R_{\text{int}} = 0.060$
Absorption correction: multi-scan	$\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 2.7^\circ$
(<i>CrystalClear-SM Expert</i> ; Rigaku, 2012)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.724, T_{\text{max}} = 1.000$	$k = -28 \rightarrow 28$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.4055P]$
$wR(F^2) = 0.093$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3063 reflections	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
191 parameters	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
0 restraints	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S6	0.17185 (4)	0.41173 (2)	0.46144 (3)	0.02043 (11)
O6	0.42208 (12)	0.47291 (4)	0.71480 (12)	0.0275 (2)
O63	0.70355 (13)	0.67387 (4)	0.97072 (11)	0.0288 (2)
N1	-0.06585 (14)	0.44463 (5)	0.16289 (13)	0.0227 (2)
N3	-0.25987 (15)	0.37375 (5)	-0.03578 (13)	0.0240 (2)
N7	0.01119 (14)	0.28258 (5)	0.30139 (13)	0.0211 (2)
N9	-0.21099 (14)	0.26758 (5)	0.06007 (13)	0.0226 (2)

H9	-0.2911	0.2481	-0.0214	0.027*
C2	-0.19450 (17)	0.42912 (6)	0.01862 (15)	0.0247 (3)
H6	-0.2451	0.4623	-0.0538	0.030*
C4	-0.17933 (16)	0.32957 (6)	0.07248 (15)	0.0206 (2)
C5	-0.04241 (16)	0.33841 (5)	0.22326 (14)	0.0195 (2)
C6	0.01075 (15)	0.39879 (6)	0.26754 (14)	0.0194 (2)
C8	-0.09352 (16)	0.24220 (6)	0.19916 (15)	0.0225 (3)
H8	-0.0874	0.1993	0.2207	0.027*
C61	0.21217 (16)	0.49315 (6)	0.44829 (15)	0.0213 (2)
H61A	0.2602	0.5018	0.3537	0.026*
H61B	0.0969	0.5163	0.4312	0.026*
C62	0.35075 (16)	0.51187 (6)	0.61124 (15)	0.0207 (2)
C631	0.39980 (16)	0.57789 (6)	0.63995 (15)	0.0205 (2)
C632	0.52582 (16)	0.59345 (5)	0.79351 (15)	0.0208 (2)
H632	0.5744	0.5626	0.8745	0.025*
C633	0.57924 (17)	0.65409 (6)	0.82667 (16)	0.0230 (3)
C634	0.50351 (18)	0.69940 (6)	0.70857 (17)	0.0259 (3)
H634	0.5385	0.7410	0.7320	0.031*
C635	0.37787 (18)	0.68404 (6)	0.55762 (17)	0.0265 (3)
H635	0.3264	0.7152	0.4785	0.032*
C636	0.32641 (16)	0.62298 (6)	0.52100 (16)	0.0238 (3)
H636	0.2425	0.6123	0.4164	0.029*
C637	0.7840 (2)	0.62823 (6)	1.09270 (17)	0.0301 (3)
H63A	0.8724	0.6476	1.1886	0.045*
H63B	0.8465	0.5976	1.0440	0.045*
H63C	0.6882	0.6081	1.1291	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S6	0.02055 (17)	0.02018 (17)	0.01696 (16)	-0.00081 (10)	0.00019 (11)	-0.00014 (10)
O6	0.0294 (5)	0.0212 (5)	0.0250 (5)	-0.0002 (3)	-0.0021 (4)	0.0020 (3)
O63	0.0378 (5)	0.0234 (5)	0.0227 (5)	-0.0077 (4)	0.0053 (4)	-0.0043 (4)
N1	0.0231 (5)	0.0235 (5)	0.0196 (5)	0.0015 (4)	0.0036 (4)	0.0024 (4)
N3	0.0229 (5)	0.0282 (6)	0.0173 (5)	0.0029 (4)	0.0005 (4)	0.0022 (4)
N7	0.0203 (5)	0.0220 (5)	0.0178 (5)	0.0011 (4)	0.0009 (4)	0.0009 (4)
N9	0.0214 (5)	0.0242 (5)	0.0179 (5)	0.0001 (4)	-0.0005 (4)	-0.0024 (4)
C2	0.0250 (6)	0.0272 (7)	0.0185 (6)	0.0038 (5)	0.0016 (5)	0.0042 (5)
C4	0.0188 (5)	0.0249 (6)	0.0161 (5)	0.0011 (4)	0.0023 (4)	-0.0012 (5)
C5	0.0180 (5)	0.0233 (6)	0.0150 (5)	0.0015 (4)	0.0014 (4)	0.0006 (4)
C6	0.0179 (5)	0.0227 (6)	0.0166 (5)	0.0006 (4)	0.0038 (4)	0.0006 (4)
C8	0.0224 (6)	0.0222 (6)	0.0199 (6)	0.0004 (4)	0.0019 (4)	0.0000 (5)
C61	0.0206 (5)	0.0209 (6)	0.0203 (6)	-0.0011 (4)	0.0030 (5)	-0.0002 (4)
C62	0.0183 (5)	0.0225 (6)	0.0204 (6)	0.0000 (4)	0.0046 (4)	-0.0003 (4)
C631	0.0187 (5)	0.0219 (6)	0.0210 (6)	0.0000 (4)	0.0060 (4)	-0.0006 (4)
C632	0.0229 (6)	0.0202 (6)	0.0195 (6)	0.0003 (4)	0.0065 (5)	-0.0007 (4)
C633	0.0248 (6)	0.0240 (6)	0.0216 (6)	-0.0028 (5)	0.0091 (5)	-0.0030 (5)
C634	0.0298 (6)	0.0184 (6)	0.0312 (7)	-0.0018 (5)	0.0118 (5)	-0.0006 (5)

C635	0.0262 (6)	0.0228 (6)	0.0302 (7)	0.0021 (5)	0.0082 (5)	0.0053 (5)
C636	0.0208 (6)	0.0247 (7)	0.0241 (6)	0.0001 (4)	0.0042 (5)	0.0026 (5)
C637	0.0350 (7)	0.0315 (7)	0.0209 (6)	-0.0054 (5)	0.0039 (5)	-0.0024 (5)

Geometric parameters (Å, °)

S6—C6	1.7477 (12)	C61—C62	1.5162 (16)
S6—C61	1.8109 (13)	C61—H61A	0.9900
O6—C62	1.2219 (15)	C61—H61B	0.9900
O63—C633	1.3669 (15)	C62—C631	1.4887 (17)
O63—C637	1.4293 (17)	C631—C636	1.3949 (17)
N1—C6	1.3446 (16)	C631—C632	1.4025 (17)
N1—C2	1.3566 (16)	C632—C633	1.3871 (17)
N3—C2	1.3342 (17)	C632—H632	0.9500
N3—C4	1.3416 (16)	C633—C634	1.3975 (18)
N7—C8	1.3206 (16)	C634—C635	1.3846 (19)
N7—C5	1.3855 (15)	C634—H634	0.9500
N9—C8	1.3612 (15)	C635—C636	1.3963 (18)
N9—C4	1.3716 (16)	C635—H635	0.9500
N9—H9	0.8800	C636—H636	0.9500
C2—H6	0.9500	C637—H63A	0.9800
C4—C5	1.3954 (16)	C637—H63B	0.9800
C5—C6	1.3950 (17)	C637—H63C	0.9800
C8—H8	0.9500		
C6—S6—C61	100.77 (6)	H61A—C61—H61B	108.5
C633—O63—C637	116.88 (10)	O6—C62—C631	121.28 (11)
C6—N1—C2	117.22 (11)	O6—C62—C61	119.95 (11)
C2—N3—C4	111.58 (11)	C631—C62—C61	118.75 (10)
C8—N7—C5	103.95 (10)	C636—C631—C632	120.52 (11)
C8—N9—C4	106.19 (10)	C636—C631—C62	122.49 (11)
C8—N9—H9	126.9	C632—C631—C62	116.99 (11)
C4—N9—H9	126.9	C633—C632—C631	119.72 (12)
N3—C2—N1	129.01 (12)	C633—C632—H632	120.1
N3—C2—H6	115.5	C631—C632—H632	120.1
N1—C2—H6	115.5	O63—C633—C632	124.33 (12)
N3—C4—N9	128.37 (11)	O63—C633—C634	115.92 (11)
N3—C4—C5	125.80 (12)	C632—C633—C634	119.75 (12)
N9—C4—C5	105.83 (10)	C635—C634—C633	120.46 (12)
N7—C5—C6	132.92 (11)	C635—C634—H634	119.8
N7—C5—C4	110.17 (11)	C633—C634—H634	119.8
C6—C5—C4	116.90 (11)	C634—C635—C636	120.36 (12)
N1—C6—C5	119.44 (11)	C634—C635—H635	119.8
N1—C6—S6	122.55 (10)	C636—C635—H635	119.8
C5—C6—S6	117.99 (9)	C631—C636—C635	119.17 (12)
N7—C8—N9	113.85 (11)	C631—C636—H636	120.4
N7—C8—H8	123.1	C635—C636—H636	120.4
N9—C8—H8	123.1	O63—C637—H63A	109.5

C62—C61—S6	107.14 (8)	O63—C637—H63B	109.5
C62—C61—H61A	110.3	H63A—C637—H63B	109.5
S6—C61—H61A	110.3	O63—C637—H63C	109.5
C62—C61—H61B	110.3	H63A—C637—H63C	109.5
S6—C61—H61B	110.3	H63B—C637—H63C	109.5
C4—N3—C2—N1	-0.95 (19)	C4—N9—C8—N7	0.34 (14)
C6—N1—C2—N3	0.9 (2)	C6—S6—C61—C62	179.54 (8)
C2—N3—C4—N9	179.68 (12)	S6—C61—C62—O6	5.56 (14)
C2—N3—C4—C5	-0.74 (18)	S6—C61—C62—C631	-175.65 (9)
C8—N9—C4—N3	178.96 (12)	O6—C62—C631—C636	177.18 (11)
C8—N9—C4—C5	-0.68 (13)	C61—C62—C631—C636	-1.59 (17)
C8—N7—C5—C6	178.02 (13)	O6—C62—C631—C632	-2.42 (17)
C8—N7—C5—C4	-0.60 (13)	C61—C62—C631—C632	178.81 (10)
N3—C4—C5—N7	-178.84 (11)	C636—C631—C632—C633	-0.64 (18)
N9—C4—C5—N7	0.81 (13)	C62—C631—C632—C633	178.98 (11)
N3—C4—C5—C6	2.29 (18)	C637—O63—C633—C632	0.86 (17)
N9—C4—C5—C6	-178.05 (10)	C637—O63—C633—C634	-179.47 (11)
C2—N1—C6—C5	0.84 (17)	C631—C632—C633—O63	-178.68 (11)
C2—N1—C6—S6	-177.49 (9)	C631—C632—C633—C634	1.66 (18)
N7—C5—C6—N1	179.21 (12)	O63—C633—C634—C635	179.22 (11)
C4—C5—C6—N1	-2.24 (17)	C632—C633—C634—C635	-1.09 (19)
N7—C5—C6—S6	-2.39 (18)	C633—C634—C635—C636	-0.5 (2)
C4—C5—C6—S6	176.16 (8)	C632—C631—C636—C635	-0.96 (18)
C61—S6—C6—N1	-7.88 (11)	C62—C631—C636—C635	179.45 (11)
C61—S6—C6—C5	173.78 (9)	C634—C635—C636—C631	1.54 (19)
C5—N7—C8—N9	0.16 (14)		

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>
N9—H9...N7 ⁱ	0.88	1.90	2.7715 (14)	171

Symmetry code: (i) $x-1/2, -y+1/2, z-1/2$.