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ISSN 2414-3146

1-{2-Anilino-4-methyl-5-[5-methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazole-4-carbonyl]thiophen-3-yl}ethanone

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Received 2 March 2018
Accepted 8 March 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

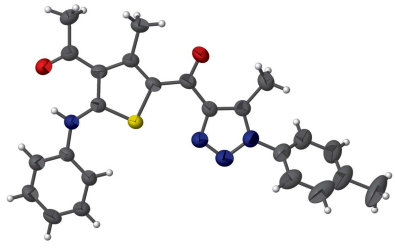
Keywords: crystal structure; 1,2,3-triazole; thiophene.

CCDC reference: 1828289

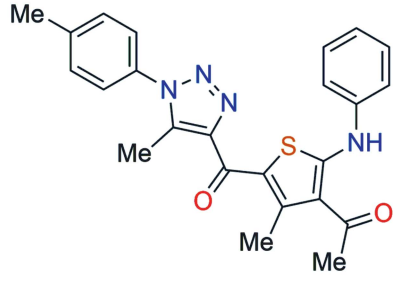
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{24}H_{22}N_4O_2S$, the dihedral angle between the triazole and thiophene rings is 4.83 (14)°. The dihedral angles between the triazole and tolyl rings and between the thiophene and phenyl rings are 48.42 (16) and 9.23 (13)°, respectively. An intramolecular N—H···O hydrogen bond closes an *S*(6) loop. In the crystal, molecules are stacked parallel to the *a*-axis direction with weak π–π interactions between adjacent thiophenyl and triazolyl groups within the stack [centroid–centroid separation = 3.9811 (16) Å].

3D view



Chemical scheme



Structure description

Heterocycles containing 1,2,3-triazole and thiophene moieties have a wide range of applications (Dheer *et al.*, 2017; Jiang & Kuang, 2013; Li *et al.*, 2016; Mancuso & Gabriele, 2014; Shafran *et al.*, 2008; Yamada *et al.*, 2018). As part of our studies in this area, we now describe the crystal structure of the title compound.

The asymmetric unit consists of one molecule of $C_{24}H_{22}N_4O_2S$ (Fig. 1). The dihedral angle between the triazole and thiophene rings is 4.83 (14)°. The dihedral angles between the triazole and tolyl rings and between the thiophene and phenyl rings are 48.42 (16) and 9.23 (13)°, respectively. An intramolecular N4—H4*A*···O2 hydrogen bond closes an *S*(6) loop (Table 1). In the crystal, the molecules are stacked parallel to the *a*-axis direction

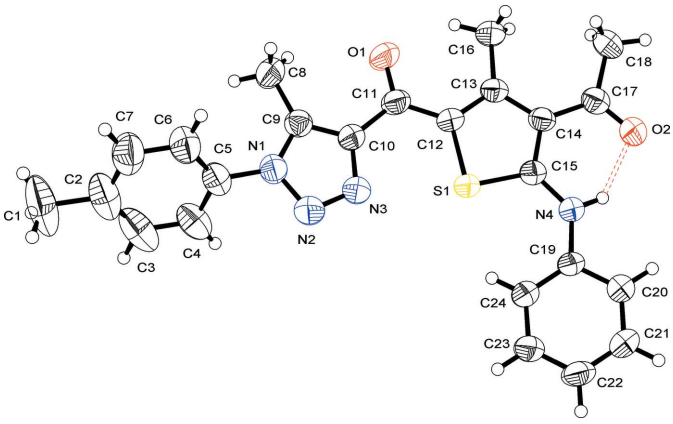


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the intramolecular N—H···O hydrogen bond (dashed lines).

with weak π–π interactions [centroid–centroid separation = 3.9811 (16) Å] between adjacent thiophenyl and triazolyl groups within the stack (Figs. 2 and 3).

Synthesis and crystallization

The title compound was obtained using a literature procedure (Mohamed *et al.*, 2017). Yellow plates were recrystallized from dimethylformamide soluton in 74% yield; m.p. 222–224°C.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

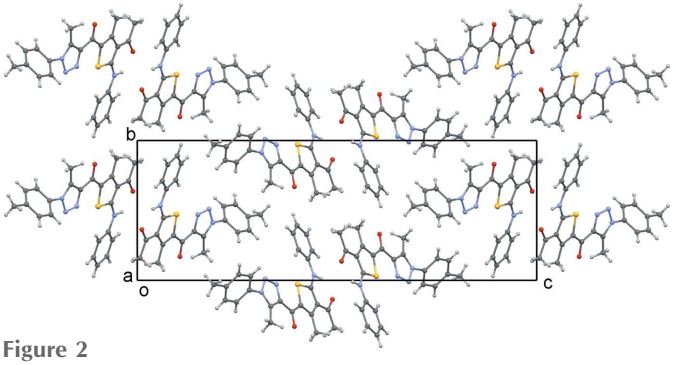


Figure 2
Crystal packing viewed down the *a* axis.

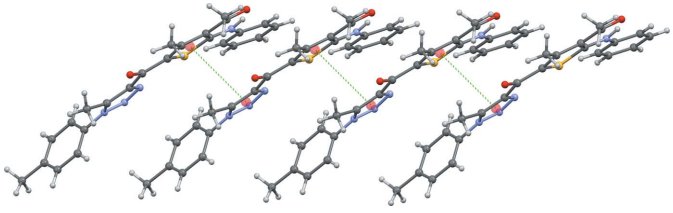


Figure 3
A segment of the crystal structure showing π–π contacts within a stack.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O2	0.86	1.91	2.605 (3)	137

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{22}N_4O_2S$
M_r	430.51
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	6.2938 (5), 10.9254 (9), 31.229 (4)
β (°)	90.221 (8)
V (Å^3)	2147.4 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.60 × 0.15 × 0.06
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.993, 0.998
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18565, 5355, 2925
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.061, 0.150, 1.03
No. of reflections	5355
No. of parameters	284
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.23

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Funding information

The project was supported by King Saud University, Deanship of Scientific Research, Research Chairs and Cardiff University.

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full crystallographic data

IUCrData (2018). **3**, x180402 [https://doi.org/10.1107/S2414314618004029]

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Crystal data

$C_{24}H_{22}N_4O_2S$
M_r = 430.51
Monoclinic, $P2_1/c$
a = 6.2938 (5) Å
b = 10.9254 (9) Å
c = 31.229 (4) Å
β = 90.221 (8)°
V = 2147.4 (4) Å^3
Z = 4
$F(000)$ = 904
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3306 reflections
θ = 3.7–25.6°
μ = 0.18 mm^{-1}
T = 296 K
Plate, yellow
0.60 × 0.15 × 0.06 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.993, T_{max} = 0.998
18565 measured reflections
5355 independent reflections
2925 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 30.0°, θ_{min} = 3.5°
h = −8→7
k = −14→15
l = −42→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.150
S = 1.03
5355 reflections
284 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.7067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

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

Refinement. All hydrogen atoms were placed in calculated positions and refined using a riding model. Aromatic C—H distances were set to 0.93\%A and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methyl groups were allowed to rotate about the C—C bond and C—H distances were set to 0.96\%A with U(iso) set to 1.5 times the U_{eq} for the C atoms to which they are bonded. The N—H bond was set to 0.86 Å and U_{iso}(H) set to 1.2 times U_{eq} (N).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0844 (6)	0.4701 (5)	0.30830 (15)	0.147 (2)
H1A	1.108519	0.393718	0.322722	0.221*
H1B	1.052358	0.532344	0.328987	0.221*
H1C	1.209563	0.492748	0.292718	0.221*
C2	0.8982 (5)	0.4565 (5)	0.27729 (13)	0.0941 (12)
C3	0.8627 (5)	0.5421 (4)	0.24562 (13)	0.0975 (13)
H3	0.951860	0.609790	0.243839	0.117*
C4	0.6972 (5)	0.5300 (3)	0.21623 (11)	0.0781 (9)
H4	0.675965	0.588220	0.194905	0.094*
C5	0.5657 (4)	0.4299 (3)	0.21949 (10)	0.0599 (7)
C6	0.5955 (5)	0.3451 (3)	0.25146 (11)	0.0759 (9)
H6	0.503424	0.278965	0.254083	0.091*
C7	0.7638 (5)	0.3589 (4)	0.27974 (12)	0.0909 (11)
H7	0.785641	0.300306	0.300890	0.109*
C8	0.4691 (4)	0.1979 (2)	0.16645 (10)	0.0658 (8)
H8A	0.610090	0.213815	0.176877	0.099*
H8B	0.476556	0.165169	0.137965	0.099*
H8C	0.400558	0.139825	0.184882	0.099*
C9	0.3448 (4)	0.3143 (2)	0.16587 (9)	0.0506 (6)
C10	0.1699 (4)	0.3507 (2)	0.14252 (9)	0.0499 (6)
C11	0.0454 (4)	0.2756 (2)	0.11238 (9)	0.0544 (7)
C12	−0.1452 (4)	0.3207 (2)	0.09090 (8)	0.0485 (6)
C13	−0.2792 (4)	0.2570 (2)	0.06385 (8)	0.0483 (6)
C14	−0.4553 (4)	0.3276 (2)	0.04919 (8)	0.0468 (6)
C15	−0.4475 (4)	0.4479 (2)	0.06554 (8)	0.0462 (6)
C16	−0.2392 (5)	0.1256 (2)	0.05188 (12)	0.0774 (10)
H16A	−0.099602	0.102095	0.061276	0.116*
H16B	−0.249296	0.116666	0.021362	0.116*
H16C	−0.343038	0.074289	0.065371	0.116*
C17	−0.6339 (4)	0.2894 (2)	0.02206 (9)	0.0535 (7)
C18	−0.6614 (4)	0.1593 (2)	0.00682 (11)	0.0708 (8)
H18A	−0.792619	0.152184	−0.008755	0.106*
H18B	−0.663793	0.105202	0.031040	0.106*
H18C	−0.545254	0.137656	−0.011533	0.106*
C19	−0.6221 (4)	0.6541 (2)	0.07278 (8)	0.0483 (6)

C20	−0.8126 (4)	0.7101 (2)	0.06251 (10)	0.0622 (8)
H20	−0.914276	0.668419	0.046483	0.075*
C21	−0.8514 (4)	0.8282 (3)	0.07617 (11)	0.0720 (9)
H21	−0.979294	0.865810	0.069033	0.086*
C22	−0.7045 (5)	0.8909 (2)	0.10002 (10)	0.0691 (8)
H22	−0.732975	0.969785	0.109568	0.083*
C23	−0.5159 (5)	0.8359 (2)	0.10959 (10)	0.0708 (9)
H23	−0.414335	0.878505	0.125337	0.085*
C24	−0.4730 (4)	0.7178 (2)	0.09628 (10)	0.0653 (8)
H24	−0.343707	0.681488	0.103168	0.078*
N1	0.3972 (3)	0.4139 (2)	0.18886 (7)	0.0557 (6)
N2	0.2643 (4)	0.5101 (2)	0.17970 (8)	0.0674 (7)
N3	0.1272 (3)	0.4702 (2)	0.15169 (8)	0.0614 (6)
N4	−0.5960 (3)	0.53417 (17)	0.05747 (7)	0.0519 (5)
H4A	−0.692643	0.511443	0.039618	0.062*
O1	0.1094 (3)	0.16977 (17)	0.10657 (8)	0.0850 (7)
O2	−0.7730 (3)	0.36351 (17)	0.01127 (7)	0.0678 (6)
S1	−0.23163 (9)	0.47131 (5)	0.09830 (2)	0.0503 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.070 (2)	0.251 (6)	0.121 (4)	−0.001 (3)	−0.031 (2)	−0.071 (4)
C2	0.0587 (18)	0.149 (4)	0.075 (3)	−0.004 (2)	−0.0041 (17)	−0.040 (3)
C3	0.075 (2)	0.134 (3)	0.084 (3)	−0.040 (2)	0.018 (2)	−0.044 (3)
C4	0.0793 (19)	0.090 (2)	0.066 (2)	−0.0208 (18)	0.0045 (16)	−0.0187 (18)
C5	0.0502 (14)	0.0720 (18)	0.058 (2)	−0.0035 (14)	0.0001 (13)	−0.0134 (16)
C6	0.0725 (18)	0.087 (2)	0.068 (2)	−0.0062 (17)	−0.0122 (16)	−0.0021 (19)
C7	0.084 (2)	0.115 (3)	0.074 (3)	0.014 (2)	−0.0183 (19)	−0.013 (2)
C8	0.0622 (16)	0.0630 (17)	0.072 (2)	0.0132 (14)	−0.0087 (14)	−0.0003 (15)
C9	0.0525 (14)	0.0490 (14)	0.0504 (17)	0.0010 (12)	0.0005 (11)	−0.0017 (12)
C10	0.0511 (13)	0.0455 (14)	0.0529 (17)	0.0047 (11)	−0.0030 (11)	−0.0017 (12)
C11	0.0641 (15)	0.0423 (14)	0.0567 (19)	0.0090 (12)	−0.0034 (13)	−0.0030 (12)
C12	0.0531 (13)	0.0364 (12)	0.0558 (18)	0.0043 (11)	−0.0017 (12)	0.0002 (12)
C13	0.0536 (13)	0.0386 (12)	0.0528 (17)	0.0000 (11)	0.0009 (11)	−0.0038 (11)
C14	0.0504 (13)	0.0383 (12)	0.0518 (17)	−0.0019 (11)	0.0007 (11)	−0.0044 (11)
C15	0.0492 (13)	0.0400 (13)	0.0494 (17)	−0.0005 (11)	−0.0014 (11)	0.0011 (11)
C16	0.0778 (19)	0.0449 (15)	0.109 (3)	0.0109 (14)	−0.0271 (18)	−0.0228 (17)
C17	0.0557 (14)	0.0493 (15)	0.0555 (18)	−0.0039 (13)	0.0006 (12)	−0.0054 (13)
C18	0.0740 (18)	0.0581 (17)	0.080 (2)	−0.0079 (14)	−0.0177 (16)	−0.0171 (16)
C19	0.0536 (14)	0.0363 (12)	0.0550 (17)	0.0052 (11)	−0.0055 (11)	−0.0012 (11)
C20	0.0556 (15)	0.0513 (15)	0.080 (2)	0.0044 (13)	−0.0134 (14)	−0.0078 (14)
C21	0.0632 (17)	0.0551 (17)	0.097 (3)	0.0184 (14)	−0.0155 (16)	−0.0080 (17)
C22	0.086 (2)	0.0438 (14)	0.078 (2)	0.0183 (15)	−0.0109 (16)	−0.0106 (15)
C23	0.084 (2)	0.0466 (15)	0.081 (2)	0.0089 (14)	−0.0286 (16)	−0.0139 (15)
C24	0.0674 (16)	0.0465 (15)	0.082 (2)	0.0116 (13)	−0.0253 (15)	−0.0088 (14)
N1	0.0520 (11)	0.0577 (13)	0.0573 (16)	0.0025 (11)	−0.0050 (10)	−0.0065 (11)
N2	0.0664 (14)	0.0566 (14)	0.0792 (19)	0.0067 (12)	−0.0090 (12)	−0.0127 (13)

N3	0.0627 (13)	0.0518 (13)	0.0696 (17)	0.0071 (11)	−0.0129 (12)	−0.0119 (12)
N4	0.0520 (11)	0.0410 (11)	0.0625 (16)	0.0040 (10)	−0.0124 (10)	−0.0044 (10)
O1	0.0985 (15)	0.0523 (12)	0.1039 (19)	0.0276 (11)	−0.0425 (13)	−0.0197 (12)
O2	0.0611 (11)	0.0579 (11)	0.0842 (16)	0.0031 (9)	−0.0205 (10)	−0.0145 (10)
S1	0.0548 (4)	0.0376 (3)	0.0585 (5)	0.0043 (3)	−0.0103 (3)	−0.0054 (3)

Geometric parameters (Å, º)

C1—C2	1.525 (5)	C13—C16	1.504 (3)
C1—H1A	0.9600	C14—C15	1.411 (3)
C1—H1B	0.9600	C14—C17	1.465 (3)
C1—H1C	0.9600	C15—N4	1.351 (3)
C2—C7	1.363 (5)	C15—S1	1.717 (2)
C2—C3	1.379 (5)	C16—H16A	0.9600
C3—C4	1.392 (5)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600
C4—C5	1.376 (4)	C17—O2	1.238 (3)
C4—H4	0.9300	C17—C18	1.509 (3)
C5—C6	1.374 (4)	C18—H18A	0.9600
C5—N1	1.436 (3)	C18—H18B	0.9600
C6—C7	1.385 (4)	C18—H18C	0.9600
C6—H6	0.9300	C19—C24	1.378 (3)
C7—H7	0.9300	C19—C20	1.383 (3)
C8—C9	1.493 (3)	C19—N4	1.404 (3)
C8—H8A	0.9600	C20—C21	1.381 (4)
C8—H8B	0.9600	C20—H20	0.9300
C8—H8C	0.9600	C21—C22	1.368 (4)
C9—N1	1.344 (3)	C21—H21	0.9300
C9—C10	1.377 (3)	C22—C23	1.362 (4)
C10—N3	1.363 (3)	C22—H22	0.9300
C10—C11	1.473 (4)	C23—C24	1.382 (4)
C11—O1	1.237 (3)	C23—H23	0.9300
C11—C12	1.458 (3)	C24—H24	0.9300
C12—C13	1.380 (3)	N1—N2	1.373 (3)
C12—S1	1.748 (2)	N2—N3	1.302 (3)
C13—C14	1.425 (3)	N4—H4A	0.8600
C2—C1—H1A	109.5	C13—C14—C17	128.7 (2)
C2—C1—H1B	109.5	N4—C15—C14	124.0 (2)
H1A—C1—H1B	109.5	N4—C15—S1	123.54 (18)
C2—C1—H1C	109.5	C14—C15—S1	112.40 (17)
H1A—C1—H1C	109.5	C13—C16—H16A	109.5
H1B—C1—H1C	109.5	C13—C16—H16B	109.5
C7—C2—C3	118.1 (3)	H16A—C16—H16B	109.5
C7—C2—C1	121.1 (5)	C13—C16—H16C	109.5
C3—C2—C1	120.8 (4)	H16A—C16—H16C	109.5
C2—C3—C4	121.8 (3)	H16B—C16—H16C	109.5
C2—C3—H3	119.1	O2—C17—C14	120.7 (2)

C4—C3—H3	119.1	O2—C17—C18	116.8 (2)
C5—C4—C3	118.4 (4)	C14—C17—C18	122.5 (2)
C5—C4—H4	120.8	C17—C18—H18A	109.5
C3—C4—H4	120.8	C17—C18—H18B	109.5
C6—C5—C4	120.6 (3)	H18A—C18—H18B	109.5
C6—C5—N1	120.0 (3)	C17—C18—H18C	109.5
C4—C5—N1	119.4 (3)	H18A—C18—H18C	109.5
C5—C6—C7	119.4 (3)	H18B—C18—H18C	109.5
C5—C6—H6	120.3	C24—C19—C20	119.2 (2)
C7—C6—H6	120.3	C24—C19—N4	124.9 (2)
C2—C7—C6	121.5 (4)	C20—C19—N4	115.9 (2)
C2—C7—H7	119.2	C21—C20—C19	119.7 (3)
C6—C7—H7	119.2	C21—C20—H20	120.1
C9—C8—H8A	109.5	C19—C20—H20	120.1
C9—C8—H8B	109.5	C22—C21—C20	121.0 (3)
H8A—C8—H8B	109.5	C22—C21—H21	119.5
C9—C8—H8C	109.5	C20—C21—H21	119.5
H8A—C8—H8C	109.5	C23—C22—C21	119.0 (3)
H8B—C8—H8C	109.5	C23—C22—H22	120.5
N1—C9—C10	104.1 (2)	C21—C22—H22	120.5
N1—C9—C8	123.7 (2)	C22—C23—C24	121.1 (3)
C10—C9—C8	132.1 (2)	C22—C23—H23	119.4
N3—C10—C9	108.9 (2)	C24—C23—H23	119.4
N3—C10—C11	124.3 (2)	C19—C24—C23	119.9 (2)
C9—C10—C11	126.8 (2)	C19—C24—H24	120.1
O1—C11—C12	121.1 (2)	C23—C24—H24	120.1
O1—C11—C10	116.2 (2)	C9—N1—N2	111.1 (2)
C12—C11—C10	122.7 (2)	C9—N1—C5	129.3 (2)
C13—C12—C11	127.6 (2)	N2—N1—C5	119.6 (2)
C13—C12—S1	111.51 (17)	N3—N2—N1	106.6 (2)
C11—C12—S1	120.89 (19)	N2—N3—C10	109.4 (2)
C12—C13—C14	113.3 (2)	C15—N4—C19	132.0 (2)
C12—C13—C16	122.1 (2)	C15—N4—H4A	114.0
C14—C13—C16	124.6 (2)	C19—N4—H4A	114.0
C15—C14—C13	111.2 (2)	C15—S1—C12	91.53 (11)
C15—C14—C17	120.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O2	0.86	1.91	2.605 (3)	137