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Ethyl 2-anilino-4-methyl-5-[5-methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazole-4-carbonyl]thiophene-3-carboxylate

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

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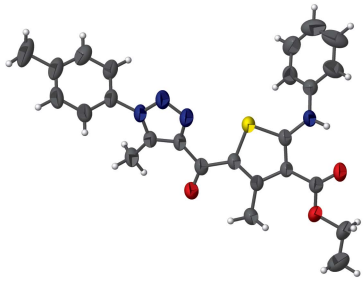
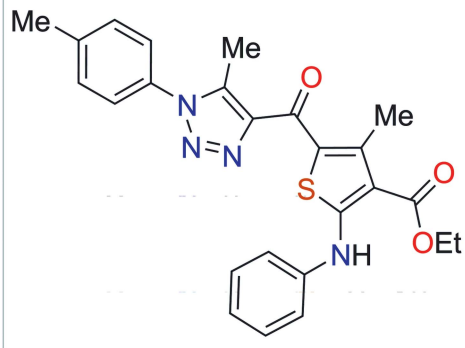
Structural data: full structural data are available from iucrdata.iucr.org

The conformation of the title compound, $C_{25}H_{24}N_4O_3S$, is influenced by an intramolecular N—H···O hydrogen bond, which generates an *S*(6) ring. The twist angles between the planes through the toluyl, methyltriazole, thiophene and phenyl rings are 60.1 (1), 33.5 (1) and 39.9 (1)°, respectively. In the crystal, molecules are stacked along the *a*-axis direction with weak aromatic π–π stacking interactions occurring between the thiophene rings [centroid-to-centroid distance = 3.7285 (15) Å].

3D view



Chemical scheme



Structure description

Substituted 2-aminothiophenes are found in numerous biologically active compounds including olanzapine as an antipsychotic drug and tinoridine as a potent nonsteroidal anti-inflammatory drug (Al-Taisan *et al.*, 2010; Huang & Dömling, 2011; Wardakhan *et al.*, 2016). As part of our studies of similar systems, we now describe the structure of the title compound.

The asymmetric unit comprises one molecule of $C_{25}H_{24}N_4O_3S$ (Fig. 1). An intramolecular N—H···O hydrogen bond occurs in the molecule (Table 1) and the twist angles between the planes through the toluyl, methyltriazole, thiophene and phenyl rings are 60.1 (1)°, 33.5 (1)° and 39.9 (1)° respectively. In the crystal, molecules are stacked along the *a*-axis and π–π type interactions involving thiophene groups of neighbouring

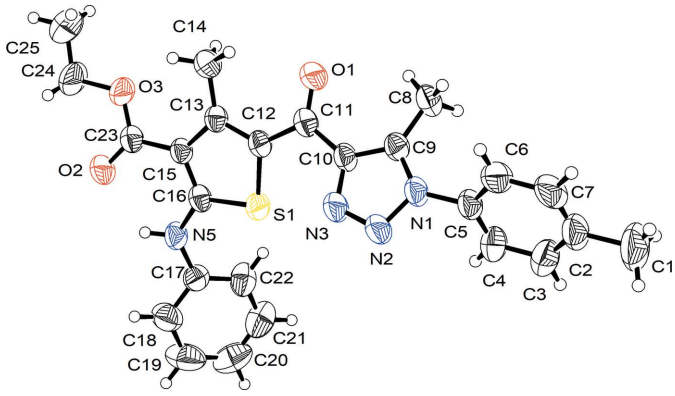


Figure 1
The molecular structure of the title compound, showing 50% displacement ellipsoids.

molecules with centroid-to-centroid distances of 3.7285 (15) Å are observed (Fig. 2); the pairs are related by a twofold rotation axis.

Synthesis and crystallization

The title compound was synthesized by a literature procedure (Mohamed *et al.*, 2017) in 78% yield and recrystallized from dimethylformamide solution as yellow plates, m.p. 472–473 K.

Refinement

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

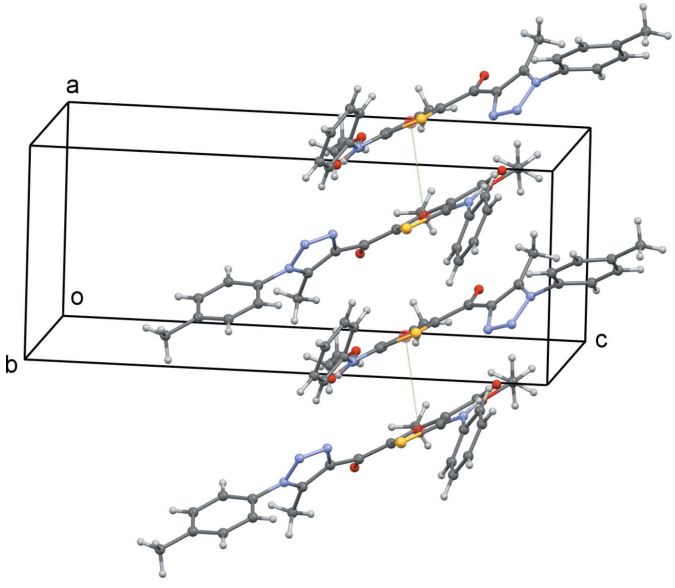


Figure 2
A segment of the crystal structure showing thiophene π–π contacts as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O2	0.86	2.08	2.704 (3)	129

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{24}N_4O_3S$
M_r	460.54
Crystal system, space group	Monoclinic, $P2/c$
Temperature (K)	293
a, b, c (Å)	8.3287 (7), 13.8956 (9), 20.3124 (15)
β (°)	90.635 (8)
V (Å^3)	2350.7 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.23 × 0.15 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.995, 0.999
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22546, 5978, 2688
R_{int}	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.700
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.182, 1.01
No. of reflections	5978
No. of parameters	302
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.27

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).

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full crystallographic data

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Crystal data

$C_{25}H_{24}N_4O_3S$
M_r = 460.54
Monoclinic, $P2/c$
a = 8.3287 (7) Å
b = 13.8956 (9) Å
c = 20.3124 (15) Å
β = 90.635 (8)°
V = 2350.7 (3) Å^3
Z = 4
$F(000)$ = 968
D_x = 1.301 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3069 reflections
θ = 3.9–24.4°
μ = 0.17 mm^{-1}
T = 293 K
Plate, yellow
0.23 × 0.15 × 0.04 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} = 0.995, T_{max} = 0.999
22546 measured reflections
5978 independent reflections
2688 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 29.8°, θ_{min} = 1.5°
h = −8→11
k = −19→18
l = −27→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.182
S = 1.01
5978 reflections
302 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.1629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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. Non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C), and were allowed to spin about the C—C bond. Methylene C—H bonds were fixed at 0.97 Å with displacement parameters 1.2 times U_{eq}(C). The N—H bond was fixed at 0.86 Å and aromatic C—H distances were set to 0.93 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2351 (6)	0.5726 (3)	−0.2019 (2)	0.1272 (19)
H1A	0.258516	0.607548	−0.241464	0.191*
H1B	0.121086	0.571410	−0.195501	0.191*
H1C	0.274461	0.507974	−0.205703	0.191*
C2	0.3162 (4)	0.6218 (3)	−0.14350 (19)	0.0806 (11)
C3	0.3240 (4)	0.5779 (3)	−0.08255 (19)	0.0773 (10)
H3	0.280124	0.516873	−0.077300	0.093*
C4	0.3951 (4)	0.6227 (2)	−0.02960 (16)	0.0682 (9)
H4	0.398191	0.592515	0.011252	0.082*
C5	0.4618 (4)	0.7124 (2)	−0.03719 (15)	0.0573 (8)
C6	0.4602 (5)	0.7578 (2)	−0.09710 (16)	0.0738 (10)
H6	0.507335	0.817946	−0.102273	0.089*
C7	0.3861 (5)	0.7112 (3)	−0.15004 (17)	0.0856 (12)
H7	0.383682	0.741238	−0.190945	0.103*
C8	0.3672 (3)	0.9046 (2)	0.02623 (15)	0.0606 (8)
H8A	0.390832	0.931514	−0.016115	0.091*
H8B	0.353249	0.955629	0.057517	0.091*
H8C	0.270483	0.867268	0.023214	0.091*
C9	0.5025 (3)	0.8417 (2)	0.04803 (14)	0.0499 (7)
C10	0.6094 (3)	0.8475 (2)	0.09995 (14)	0.0499 (7)
C11	0.6279 (3)	0.9260 (2)	0.14862 (14)	0.0523 (7)
C12	0.7123 (3)	0.90717 (19)	0.21113 (13)	0.0478 (7)
C13	0.7711 (3)	0.97434 (18)	0.25536 (13)	0.0462 (7)
C14	0.7598 (4)	1.0808 (2)	0.24459 (15)	0.0652 (9)
H14A	0.748681	1.093725	0.198343	0.098*
H14B	0.855405	1.111218	0.261266	0.098*
H14C	0.668146	1.105577	0.267262	0.098*
C15	0.8426 (3)	0.92958 (18)	0.31215 (13)	0.0452 (6)
C16	0.8296 (3)	0.8298 (2)	0.31015 (13)	0.0492 (7)
C17	0.8438 (4)	0.6707 (2)	0.36650 (14)	0.0543 (7)
C18	0.9483 (4)	0.6112 (2)	0.39992 (19)	0.0785 (10)
H18	1.046890	0.634573	0.414740	0.094*
C19	0.9063 (5)	0.5164 (3)	0.4114 (2)	0.1003 (14)
H19	0.976830	0.476175	0.434132	0.120*
C20	0.7604 (6)	0.4812 (3)	0.3894 (2)	0.0944 (12)
H20	0.733104	0.417163	0.396539	0.113*
C21	0.6571 (5)	0.5408 (3)	0.35733 (18)	0.0844 (11)
H21	0.558510	0.517401	0.342538	0.101*
C22	0.6966 (4)	0.6350 (2)	0.34652 (15)	0.0690 (9)

H22	0.623431	0.675404	0.325436	0.083*
C23	0.9240 (3)	0.9763 (2)	0.36794 (14)	0.0500 (7)
C24	0.9832 (5)	1.1200 (3)	0.42540 (19)	0.0979 (14)
H24A	0.942386	1.098416	0.467452	0.117*
H24B	1.096991	1.105427	0.423970	0.117*
C25	0.9584 (6)	1.2224 (3)	0.4184 (2)	0.1055 (15)
H25A	0.993383	1.242598	0.375645	0.158*
H25B	1.019087	1.255818	0.451680	0.158*
H25C	0.846424	1.236812	0.423043	0.158*
N1	0.5376 (3)	0.75785 (17)	0.01888 (11)	0.0533 (6)
N2	0.6622 (3)	0.71189 (17)	0.05061 (13)	0.0659 (7)
N3	0.7040 (3)	0.76756 (18)	0.09930 (13)	0.0638 (7)
N5	0.8863 (3)	0.76760 (15)	0.35745 (11)	0.0556 (6)
H5	0.956005	0.790616	0.384744	0.067*
O1	0.5702 (3)	1.00550 (14)	0.13552 (10)	0.0701 (6)
O2	1.0056 (2)	0.93309 (14)	0.40814 (10)	0.0633 (6)
O3	0.8992 (3)	1.07044 (14)	0.37197 (10)	0.0687 (6)
S1	0.74326 (9)	0.78984 (5)	0.23839 (4)	0.0566 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.128 (4)	0.167 (4)	0.085 (3)	0.025 (3)	−0.044 (3)	−0.059 (3)
C2	0.078 (2)	0.101 (3)	0.062 (2)	0.022 (2)	−0.022 (2)	−0.030 (2)
C3	0.075 (2)	0.089 (2)	0.068 (3)	−0.0077 (18)	−0.005 (2)	−0.024 (2)
C4	0.072 (2)	0.084 (2)	0.049 (2)	−0.0071 (17)	−0.0067 (17)	−0.0090 (17)
C5	0.0613 (18)	0.0681 (19)	0.0421 (18)	0.0094 (15)	−0.0116 (15)	−0.0086 (15)
C6	0.104 (3)	0.069 (2)	0.048 (2)	0.0157 (18)	−0.013 (2)	−0.0028 (16)
C7	0.119 (3)	0.094 (3)	0.043 (2)	0.038 (2)	−0.020 (2)	−0.0071 (19)
C8	0.0534 (17)	0.080 (2)	0.0483 (18)	0.0117 (15)	−0.0090 (15)	−0.0020 (15)
C9	0.0532 (16)	0.0578 (17)	0.0387 (16)	0.0019 (13)	−0.0038 (14)	0.0015 (13)
C10	0.0501 (15)	0.0605 (17)	0.0389 (16)	0.0035 (13)	−0.0093 (14)	−0.0008 (13)
C11	0.0504 (16)	0.0618 (18)	0.0446 (17)	−0.0007 (13)	−0.0066 (14)	0.0028 (14)
C12	0.0482 (15)	0.0560 (16)	0.0389 (16)	0.0013 (12)	−0.0061 (13)	0.0013 (12)
C13	0.0480 (15)	0.0530 (16)	0.0376 (16)	−0.0030 (12)	−0.0030 (13)	0.0003 (12)
C14	0.082 (2)	0.0602 (18)	0.053 (2)	0.0001 (15)	−0.0175 (18)	0.0064 (14)
C15	0.0477 (15)	0.0510 (15)	0.0368 (15)	−0.0009 (12)	−0.0062 (13)	0.0003 (12)
C16	0.0487 (15)	0.0592 (17)	0.0395 (16)	−0.0015 (13)	−0.0062 (13)	0.0043 (13)
C17	0.0642 (18)	0.0537 (16)	0.0450 (18)	−0.0015 (14)	−0.0017 (15)	0.0010 (14)
C18	0.068 (2)	0.067 (2)	0.100 (3)	0.0027 (17)	−0.006 (2)	0.018 (2)
C19	0.092 (3)	0.067 (2)	0.142 (4)	0.015 (2)	0.018 (3)	0.032 (2)
C20	0.114 (3)	0.061 (2)	0.109 (3)	−0.016 (2)	0.035 (3)	−0.006 (2)
C21	0.104 (3)	0.088 (3)	0.061 (2)	−0.035 (2)	0.004 (2)	0.0007 (19)
C22	0.076 (2)	0.082 (2)	0.049 (2)	−0.0230 (18)	−0.0065 (17)	0.0126 (16)
C23	0.0483 (15)	0.0568 (17)	0.0448 (17)	−0.0040 (13)	−0.0046 (14)	0.0015 (14)
C24	0.139 (4)	0.076 (2)	0.078 (3)	−0.012 (2)	−0.051 (3)	−0.016 (2)
C25	0.127 (4)	0.077 (3)	0.113 (4)	−0.010 (2)	−0.020 (3)	−0.027 (2)
N1	0.0560 (14)	0.0644 (15)	0.0391 (14)	0.0047 (11)	−0.0115 (12)	−0.0036 (11)

N2	0.0747 (17)	0.0699 (16)	0.0527 (16)	0.0169 (13)	−0.0218 (14)	−0.0058 (13)
N3	0.0719 (17)	0.0690 (16)	0.0500 (16)	0.0115 (13)	−0.0211 (14)	−0.0087 (13)
N5	0.0644 (15)	0.0574 (14)	0.0446 (14)	−0.0087 (11)	−0.0173 (13)	0.0073 (11)
O1	0.0911 (15)	0.0616 (13)	0.0569 (14)	0.0122 (11)	−0.0263 (12)	−0.0016 (10)
O2	0.0708 (13)	0.0723 (13)	0.0464 (12)	0.0054 (10)	−0.0191 (11)	−0.0015 (10)
O3	0.0939 (16)	0.0550 (13)	0.0565 (14)	−0.0055 (11)	−0.0290 (12)	−0.0054 (10)
S1	0.0691 (5)	0.0553 (4)	0.0451 (5)	−0.0026 (3)	−0.0158 (4)	0.0004 (3)

Geometric parameters (Å, º)

C1—C2	1.521 (5)	C14—H14B	0.9600
C1—H1A	0.9600	C14—H14C	0.9600
C1—H1B	0.9600	C15—C16	1.391 (4)
C1—H1C	0.9600	C15—C23	1.465 (4)
C2—C7	1.379 (5)	C16—N5	1.373 (3)
C2—C3	1.381 (5)	C16—S1	1.711 (3)
C3—C4	1.372 (4)	C17—C18	1.374 (4)
C3—H3	0.9300	C17—C22	1.379 (4)
C4—C5	1.373 (4)	C17—N5	1.405 (3)
C4—H4	0.9300	C18—C19	1.383 (5)
C5—C6	1.371 (4)	C18—H18	0.9300
C5—N1	1.442 (3)	C19—C20	1.380 (5)
C6—C7	1.394 (5)	C19—H19	0.9300
C6—H6	0.9300	C20—C21	1.355 (5)
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.489 (4)	C21—C22	1.368 (4)
C8—H8A	0.9600	C21—H21	0.9300
C8—H8B	0.9600	C22—H22	0.9300
C8—H8C	0.9600	C23—O2	1.215 (3)
C9—N1	1.341 (3)	C23—O3	1.327 (3)
C9—C10	1.375 (3)	C24—C25	1.445 (5)
C10—N3	1.363 (3)	C24—O3	1.457 (3)
C10—C11	1.479 (4)	C24—H24A	0.9700
C11—O1	1.232 (3)	C24—H24B	0.9700
C11—C12	1.468 (4)	C25—H25A	0.9600
C12—C13	1.381 (4)	C25—H25B	0.9600
C12—S1	1.740 (3)	C25—H25C	0.9600
C13—C15	1.434 (3)	N1—N2	1.373 (3)
C13—C14	1.498 (4)	N2—N3	1.300 (3)
C14—H14A	0.9600	N5—H5	0.8600
C2—C1—H1A	109.5	H14B—C14—H14C	109.5
C2—C1—H1B	109.5	C16—C15—C13	112.1 (2)
H1A—C1—H1B	109.5	C16—C15—C23	120.0 (2)
C2—C1—H1C	109.5	C13—C15—C23	127.9 (2)
H1A—C1—H1C	109.5	N5—C16—C15	125.5 (2)
H1B—C1—H1C	109.5	N5—C16—S1	122.0 (2)
C7—C2—C3	117.9 (3)	C15—C16—S1	112.37 (19)

C7—C2—C1	120.9 (4)	C18—C17—C22	119.0 (3)
C3—C2—C1	121.2 (4)	C18—C17—N5	118.8 (3)
C4—C3—C2	121.2 (4)	C22—C17—N5	122.1 (3)
C4—C3—H3	119.4	C17—C18—C19	119.7 (3)
C2—C3—H3	119.4	C17—C18—H18	120.1
C3—C4—C5	119.7 (3)	C19—C18—H18	120.1
C3—C4—H4	120.1	C20—C19—C18	120.4 (3)
C5—C4—H4	120.1	C20—C19—H19	119.8
C6—C5—C4	121.2 (3)	C18—C19—H19	119.8
C6—C5—N1	119.9 (3)	C21—C20—C19	119.4 (4)
C4—C5—N1	118.9 (3)	C21—C20—H20	120.3
C5—C6—C7	118.1 (3)	C19—C20—H20	120.3
C5—C6—H6	121.0	C20—C21—C22	120.6 (3)
C7—C6—H6	121.0	C20—C21—H21	119.7
C2—C7—C6	121.9 (3)	C22—C21—H21	119.7
C2—C7—H7	119.1	C21—C22—C17	120.8 (3)
C6—C7—H7	119.1	C21—C22—H22	119.6
C9—C8—H8A	109.5	C17—C22—H22	119.6
C9—C8—H8B	109.5	O2—C23—O3	122.1 (2)
H8A—C8—H8B	109.5	O2—C23—C15	123.5 (3)
C9—C8—H8C	109.5	O3—C23—C15	114.4 (2)
H8A—C8—H8C	109.5	C25—C24—O3	108.9 (3)
H8B—C8—H8C	109.5	C25—C24—H24A	109.9
N1—C9—C10	104.3 (2)	O3—C24—H24A	109.9
N1—C9—C8	123.1 (2)	C25—C24—H24B	109.9
C10—C9—C8	132.5 (3)	O3—C24—H24B	109.9
N3—C10—C9	108.3 (2)	H24A—C24—H24B	108.3
N3—C10—C11	123.5 (2)	C24—C25—H25A	109.5
C9—C10—C11	128.1 (2)	C24—C25—H25B	109.5
O1—C11—C12	121.9 (3)	H25A—C25—H25B	109.5
O1—C11—C10	118.6 (2)	C24—C25—H25C	109.5
C12—C11—C10	119.4 (2)	H25A—C25—H25C	109.5
C13—C12—C11	127.2 (2)	H25B—C25—H25C	109.5
C13—C12—S1	112.07 (19)	C9—N1—N2	111.4 (2)
C11—C12—S1	120.7 (2)	C9—N1—C5	129.3 (2)
C12—C13—C15	111.8 (2)	N2—N1—C5	119.3 (2)
C12—C13—C14	123.4 (2)	N3—N2—N1	106.0 (2)
C15—C13—C14	124.8 (2)	N2—N3—C10	110.0 (2)
C13—C14—H14A	109.5	C16—N5—C17	127.6 (2)
C13—C14—H14B	109.5	C16—N5—H5	116.2
H14A—C14—H14B	109.5	C17—N5—H5	116.2
C13—C14—H14C	109.5	C23—O3—C24	116.0 (2)
H14A—C14—H14C	109.5	C16—S1—C12	91.50 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···O2	0.86	2.08	2.704 (3)	129