organic compounds

Ethyl 5-[6-(furan-2-yl)-1,2,4-triazolo-[3,4-*b*][1,3,4]thiadiazol-3-yl]-2,6-dimethylnicotinate

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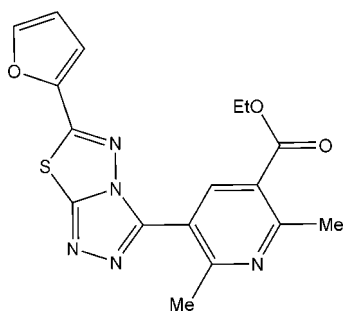Correspondence e-mail: minzhang1@yeah.net

In the title compound, $C_{17}H_{15}N_5O_3S$, the plane of the triazolo–thiadiazole system forms dihedral angles of 15.68 and 4.46° with the planes of the pyridine and furan rings, respectively. In the molecule, there is an intramolecular C—H···N interaction. The crystal structure also contains other intermolecular interactions, such as C—H···O hydrogen bonds, π–π stacking (centroid–centroid distances = 3.746 and 3.444 Å), non-bonded S···N [3.026 (2) Å] and C—H···π interactions.

Related literature

For related literature, see: Borbulevych *et al.* (1998); Bruno *et al.* (2003); Collin *et al.* (2003); Cooper & Steele (1990); Dinçer *et al.* (2005); Golgolab *et al.* (1973); Holla *et al.* (1994, 1998, 2002); Lu *et al.* (2007); Shen *et al.* (2006); Tsukuda *et al.* (1998); Wagner *et al.* (2005); Witkoaski *et al.* (1972); Zhang & Wen (1998); Özbey *et al.* (2000).

Experimental

Crystal data

$C_{17}H_{15}N_5O_3S$	$\gamma = 80.998\ (5)°$
$M_r = 369.40$	$V = 825.4\ (7)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.094\ (4)$ Å	Mo $K\alpha$ radiation
$b = 10.535\ (5)$ Å	$\mu = 0.23$ mm^{-1}
$c = 10.996\ (5)$ Å	$T = 296\ (2)$ K
$\alpha = 66.699\ (5)°$	$0.30 \times 0.30 \times 0.25$ mm
$\beta = 73.683\ (5)°$	

Data collection

Bruker SMART CCD area-detector diffractometer	4297 measured reflections
	2860 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2531 reflections with $I > 2\sigma(I)$
$T_{min} = 0.935$, $T_{max} = 0.946$	$R_{int} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	235 parameters
$wR(F^2) = 0.100$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2860 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

Cg is the centroid of the furan ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N5	0.93	2.31	2.982 (3)	128
C13—H13···O2^i	0.93	2.51	3.285 (3)	141
C17—H17A···O1^{ii}	0.96	2.56	3.424 (3)	149
C17—H17A···Cg^{iii}	0.96	3.29	4.008 (3)	134

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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supplementary materials

Ethyl 5-[6-(furan-2-yl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazol-3-yl]-2,6-dimethylnicotinate

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Comment

Antimicrobials reduce or completely block the growth and multiplication of bacteria. This has made them unique for the control of deadly infectious diseases caused by a variety of pathogens. They have transformed our ability to treat infectious diseases such as pneumonia, meningitis, tuberculosis, malaria, and AIDS. Derivatives of 1,2,4-triazole and 1,3,4-thiadiazole condensed nucleus systems are found to have diverse pharmacological activities (Collin *et al.*, 2003) such as fungicidal, insecticidal, bactericidal, herbicidal, anti-tumor (Holla *et al.*, 2002), and anti-inflammatory (Cooper & Steele, 1990), and CNS stimulant properties (Holla *et al.*, 1994). They also find applications as dyes, lubricants and analytical reagents (Zhang & Wen, 1998), antiviral agents (Witkoaski *et al.*, 1972), heterocyclic ligands (Shen *et al.*, 2006). Examples of such compounds bearing the 1,2,4-triazole moieties are fluconazole, a powerful azole antifungal agent (Tsukuda *et al.*, 1998) as well as the potent antiviral N-nucleoside ribavirin (Witkoaski *et al.*, 1972). Also, a number of 1,3,4-thiadiazoles show antibacterial properties similar to those of well known sulfonamide drugs (Golgolab *et al.*, 1973). The thiadiazole nucleus with N—C—S linkage exhibits a large number of biological activities (Holla *et al.*, 1998). Prompted by these findings and in continuation of our efforts in synthesizing some condensed bridge bioactive molecules bearing multifunctional and pharmaceutically active groups, herein, we report a new 1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole derivative which has been firstly prepared. In view of these important properties, the present single-crystal X-ray diffraction study of the title compound, (I), was carried out in order to investigate this bicyclic system and to confirm the assigned structure.

Compound (I) (Fig. 1) is composed of a fused triazolo-thiadiazole system, one pyridine ring attached to the triazole ring, the other furan ring is bonded to the thiadiazole ring, respectively. The fused triazolo-thiadiazole ring and furan ring nearly adopt coplanar form due to formation of a large π-π conjugation system. The plane of the triazolo-thiadiazole system forms dihedral angles of 15.68 and 4.46 ° with the planes of the pyridine and furan rings, respectively. Remarkably, the dihedral angle of pyridine and triazole-thiadiazole planes is significantly larger than this in the literature [1.53 ° (Dinçer *et al.*, 2005)]. This should be attributed to the steric hindrance caused by the methyl group at α-position of pyridine ring, resulting in the enlargement of dihedral angle.

Moreover, the bond distance N2—N3 (1.398 (2) Å) is in accordance with those found for structures containing the 1,2,4-triazole ring (Lu *et al.*, 2007; Bruno *et al.*, 2003), indicating that the bond distance N2—N3 is relevant to the resonance effect of fused triazole-thiadizole ring, other than the dihedral angle between the pyridine ring and a fused ring, although two molecules display different dihedral angles. Apparently, it is longer than that of 5-ammo-3-trifluoromethyl-1-H-1,2,4-triazole [1.371 Å (Borbulevych *et al.*, 1998)], because the latter contains an electron-withdrawing CF_3 group attached to the 3-position of the triazole ring. In the thiadiazole moiety, the S1—C10 (1.730 (8) Å) and S1—C11 (1.761 (8) Å) bond distances show the similar pattern as those in the literature (Dinçer *et al.*, 2005). The difference between S1—C10 and S1—C11 indicates that the bond distances mainly depend on the nature of resonance effort caused by fused triazolo-thiadiazole, rather than the aromatic ring attached to the 5-position of thiadiazole ring, because in our case, the aromatic ring is not the phenyl group, but the furan-2-yl group. The bond distances and angles of the furan ring are comparable with those in the literature (Wagner *et al.*, 2005).

supplementary materials

In the molecular structure, intramolecular C3—H3···N5 contacts lead to the formation of a five-membered ring fused with the pyridine ring. In addition, the C3—N5 distance is 2.982 (3) Å, a little shorter than that in the literature [3.140 (2)Å Özbey *et al.*, 2000)].

The structure contains two weak π-π stacking interactions. The first of them is between the triazole ring and the thiadiazol ring, its symmetry related partner at $(1 - x, -y, 1 - z)$, with a distance of 3.746 Å between the ring centroids and a perpendicular distance between the rings of 3.444 Å. The second one is between the triazole ring and the pyridine ring at $(1 - x, 1 - y, -z)$, with a distance of 3.701Å between the ring centroids and a perpendicular distance between the rings of 3.541 Å. In addition to these interactions, there are two types of intermolecular hydrogen bonds C13—H13···O2 $(1 - x, 1 - y, 1 - z)$ and C17—H17A···O1 $(1 - x, -y, 1 - z)$ which make the crystal structure to be more stable. The hydrogen-bonding geometry is listed in Table 2. Some short-contact distances are not listed in the table. Yet noteworthy, is S1···N3 $(1 - x, -y, -z)$ of 3.026 (2) Å, and a π-ring interaction at $(1 + x, y, z)$ with the distance 3.285 (9) Å between H17A and furan ring, both of them may cause steric hindrance.

Experimental

(1 mmol, 0.293 g)ethyl- 5-(4-amino-5-mercapto-4*H*-1,2,4-triazol-3-yl) −2,6-dimethylnicotinate, and (1 mmol, 0.112 g) furan-2- carboxylic acid were dissloved in 3.5 ml phosphorous oxychloride. The mixture was refluxed for 4 h, and allowed to cool to room temperature. The reaction mixture was poured into crushed ice, then, neutralized with dilute sodium bicarbonate solution. The solid separated was filtered off, washed with water, dried and recrystallized from chloroform afford pure product in a yield of 86% (m.p. 501–502 K). Single crystals suitable for X-ray analysis were obtained from chloroform by slow evaporation at room temperature. IR(v, cm^{-1}): 3101–3001 (Furan CH), 1725 (C=O), 1586–1444 (C=C, C=N), 1270 (C—S—C); ^{1}H-NMR (500 MHz, CD$_3$Cl): δ 8.82 (s, 1H, Pyridine CH), 6.67–7.70 (m, 3H, Furan CH), 4.41 (q, J=7.0 Hz, 2H, CH), 2.92 (s, 3H, Pyridine CH), 2.87 (s, 3H, Pyridine CH), 1.42 (t, J=7.0 Hz, 3H, CH);Element analysis, required for C$_{17}$H$_{15}$N$_5$O$_3$S: C 55.27, H 4.09, N 18.96%; Found: C 55.29, H 4.08, N 18.68%.

Refinement

All H atoms were placed in calculated positions, with C—H=0.93–0.97 Å, and included in the final cycles of refinement using a riding model, $U_{iso}(H) = 1.2U_{eq}(C)$.
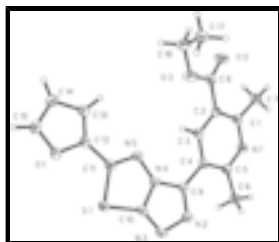
Figures

Fig. 1. The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.
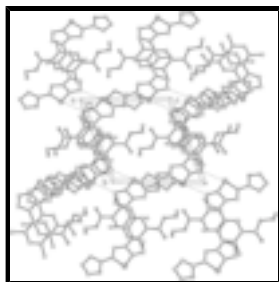
Fig. 2. The crystal packing of (I) showing the intermolecular S···N interactions.

Ethyl 5-[6-(furan-2-yl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazol-3-yl]- 2,6-dimethylnicotinate

Crystal data

$C_{17}H_{15}N_5O_3S$	$Z = 2$
$M_r = 369.40$	$F_{000} = 384$
Triclinic, $P\bar{1}$	$D_x = 1.486$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.094$ (4) Å	Cell parameters from 2601 reflections
$b = 10.535$ (5) Å	$\theta = 2.4–27.3°$
$c = 10.996$ (5) Å	$\mu = 0.23$ mm^{-1}
$\alpha = 66.699$ (5)°	$T = 296$ (2) K
$\beta = 73.683$ (5)°	Block, brown
$\gamma = 80.998$ (5)°	$0.30 \times 0.30 \times 0.25$ mm
$V = 825.4$ (7) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2860 independent reflections
Radiation source: fine-focus sealed tube	2531 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 296(2)$ K	$\theta_{max} = 25.0°$
φ and ω scans	$\theta_{min} = 2.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.935$, $T_{max} = 0.946$	$k = -12 \rightarrow 12$
4297 measured reflections	$l = -13 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.2861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{max} < 0.001$

$S = 1.06$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2860 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}
235 parameters	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.013 (3)
Secondary atom site location: difference Fourier map	

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	y	z	$U_{iso}*/U_{eq}$
N1	0.82163 (19)	0.64436 (15)	−0.06646 (15)	0.0380 (4)
N2	0.6722 (2)	0.25738 (17)	−0.06479 (16)	0.0448 (4)
N3	0.5890 (2)	0.13509 (17)	−0.02295 (17)	0.0473 (4)
N4	0.54173 (18)	0.20294 (14)	0.15000 (14)	0.0320 (3)
N5	0.46583 (19)	0.19007 (14)	0.28238 (15)	0.0349 (3)
O1	0.19535 (18)	−0.07982 (13)	0.53282 (14)	0.0469 (3)
O2	0.7628 (2)	0.63716 (16)	0.33760 (15)	0.0646 (5)
O3	0.7023 (2)	0.41744 (14)	0.41061 (14)	0.0572 (4)
S1	0.37936 (6)	−0.01525 (5)	0.23778 (5)	0.04173 (16)
C1	0.8076 (2)	0.65217 (18)	0.05519 (19)	0.0361 (4)
C2	0.7476 (2)	0.54134 (18)	0.17662 (18)	0.0337 (4)
C3	0.6956 (2)	0.42634 (18)	0.16808 (18)	0.0342 (4)
H3	0.6540	0.3523	0.2477	0.041*
C4	0.7047 (2)	0.42024 (17)	0.04290 (18)	0.0322 (4)
C5	0.7739 (2)	0.53224 (18)	−0.07487 (18)	0.0340 (4)
C6	0.8008 (3)	0.5362 (2)	−0.21624 (19)	0.0442 (5)
H6A	0.8492	0.6220	−0.2808	0.066*
H6B	0.6922	0.5286	−0.2315	0.066*
H6C	0.8782	0.4604	−0.2274	0.066*
C7	0.8615 (3)	0.7848 (2)	0.0491 (2)	0.0515 (5)
H7A	0.8978	0.8454	−0.0444	0.077*
H7B	0.9552	0.7655	0.0925	0.077*
H7C	0.7660	0.8284	0.0955	0.077*
C8	0.7393 (2)	0.54110 (19)	0.31403 (19)	0.0385 (4)
C9	0.6430 (2)	0.29802 (18)	0.03893 (18)	0.0340 (4)

C10	0.5122 (2)	0.10682 (18)	0.10579 (19)	0.0366 (4)
C11	0.3772 (2)	0.07975 (17)	0.33896 (18)	0.0352 (4)
C12	0.2798 (2)	0.04004 (17)	0.47908 (18)	0.0363 (4)
C13	0.2505 (3)	0.0984 (2)	0.5722 (2)	0.0456 (5)
H13	0.2936	0.1803	0.5607	0.055*
C14	0.1413 (3)	0.0111 (2)	0.6913 (2)	0.0501 (5)
H14	0.0985	0.0245	0.7734	0.060*
C15	0.1114 (3)	−0.0941 (2)	0.6634 (2)	0.0492 (5)
H15	0.0428	−0.1670	0.7245	0.059*
C16	0.7021 (3)	0.3943 (2)	0.5502 (2)	0.0541 (5)
H16A	0.6072	0.3378	0.6130	0.065*
H16B	0.6864	0.4822	0.5622	0.065*
C17	0.8677 (3)	0.3237 (2)	0.5807 (2)	0.0533 (5)
H17A	0.8826	0.2366	0.5692	0.080*
H17B	0.8664	0.3083	0.6730	0.080*
H17C	0.9611	0.3807	0.5195	0.080*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0420 (9)	0.0342 (8)	0.0382 (9)	−0.0062 (6)	−0.0090 (7)	−0.0126 (7)
N2	0.0553 (10)	0.0447 (9)	0.0382 (9)	−0.0173 (7)	−0.0012 (7)	−0.0207 (7)
N3	0.0605 (11)	0.0479 (9)	0.0407 (9)	−0.0211 (8)	−0.0009 (8)	−0.0249 (8)
N4	0.0370 (8)	0.0317 (7)	0.0311 (8)	−0.0054 (6)	−0.0067 (6)	−0.0152 (6)
N5	0.0403 (8)	0.0340 (8)	0.0323 (8)	−0.0061 (6)	−0.0056 (6)	−0.0148 (6)
O1	0.0598 (9)	0.0393 (7)	0.0412 (7)	−0.0186 (6)	−0.0027 (6)	−0.0150 (6)
O2	0.1001 (13)	0.0548 (9)	0.0505 (9)	−0.0282 (9)	−0.0098 (8)	−0.0283 (8)
O3	0.0959 (12)	0.0451 (8)	0.0385 (8)	−0.0120 (8)	−0.0231 (8)	−0.0158 (6)
S1	0.0537 (3)	0.0365 (3)	0.0392 (3)	−0.0147 (2)	−0.0047 (2)	−0.0183 (2)
C1	0.0346 (9)	0.0340 (9)	0.0425 (10)	−0.0045 (7)	−0.0107 (8)	−0.0151 (8)
C2	0.0320 (9)	0.0357 (9)	0.0372 (10)	−0.0038 (7)	−0.0091 (7)	−0.0164 (8)
C3	0.0358 (9)	0.0333 (9)	0.0348 (9)	−0.0067 (7)	−0.0067 (7)	−0.0135 (7)
C4	0.0326 (9)	0.0321 (9)	0.0350 (9)	−0.0032 (7)	−0.0079 (7)	−0.0151 (7)
C5	0.0324 (9)	0.0349 (9)	0.0356 (9)	−0.0013 (7)	−0.0076 (7)	−0.0147 (8)
C6	0.0554 (12)	0.0417 (10)	0.0341 (10)	−0.0073 (9)	−0.0054 (9)	−0.0144 (8)
C7	0.0695 (14)	0.0388 (11)	0.0503 (12)	−0.0178 (10)	−0.0155 (10)	−0.0146 (9)
C8	0.0373 (10)	0.0418 (10)	0.0422 (10)	−0.0069 (8)	−0.0076 (8)	−0.0214 (9)
C9	0.0373 (9)	0.0348 (9)	0.0322 (9)	−0.0064 (7)	−0.0063 (7)	−0.0145 (8)
C10	0.0438 (10)	0.0349 (9)	0.0382 (10)	−0.0068 (8)	−0.0093 (8)	−0.0196 (8)
C11	0.0395 (9)	0.0318 (9)	0.0371 (10)	−0.0041 (7)	−0.0093 (8)	−0.0151 (8)
C12	0.0402 (10)	0.0311 (9)	0.0382 (10)	−0.0058 (7)	−0.0082 (8)	−0.0129 (8)
C13	0.0534 (12)	0.0414 (11)	0.0457 (11)	−0.0087 (9)	−0.0059 (9)	−0.0218 (9)
C14	0.0568 (13)	0.0534 (12)	0.0380 (11)	−0.0045 (10)	−0.0011 (9)	−0.0211 (9)
C15	0.0525 (12)	0.0483 (11)	0.0378 (11)	−0.0122 (9)	−0.0014 (9)	−0.0095 (9)
C16	0.0740 (15)	0.0556 (13)	0.0356 (11)	−0.0058 (11)	−0.0124 (10)	−0.0195 (10)
C17	0.0652 (14)	0.0550 (12)	0.0472 (12)	−0.0138 (10)	−0.0126 (10)	−0.0236 (10)

supplementary materials

Geometric parameters (Å, °)

N1—C5	1.343 (2)	C4—C5	1.405 (2)
N1—C1	1.345 (2)	C4—C9	1.472 (2)
N2—C9	1.320 (2)	C5—C6	1.493 (3)
N2—N3	1.398 (2)	C6—H6A	0.9600
N3—C10	1.307 (2)	C6—H6B	0.9600
N4—C10	1.360 (2)	C6—H6C	0.9600
N4—N5	1.372 (2)	C7—H7A	0.9600
N4—C9	1.376 (2)	C7—H7B	0.9600
N5—C11	1.300 (2)	C7—H7C	0.9600
O1—C15	1.364 (2)	C11—C12	1.443 (3)
O1—C12	1.365 (2)	C12—C13	1.342 (3)
O2—C8	1.193 (2)	C13—C14	1.411 (3)
O3—C8	1.328 (2)	C13—H13	0.9300
O3—C16	1.455 (2)	C14—C15	1.332 (3)
S1—C10	1.7308 (19)	C14—H14	0.9300
S1—C11	1.7618 (18)	C15—H15	0.9300
C1—C2	1.401 (3)	C16—C17	1.485 (3)
C1—C7	1.499 (3)	C16—H16A	0.9700
C2—C3	1.388 (2)	C16—H16B	0.9700
C2—C8	1.492 (3)	C17—H17A	0.9600
C3—C4	1.384 (3)	C17—H17B	0.9600
C3—H3	0.9300	C17—H17C	0.9600
C5—N1—C1	121.07 (15)	O2—C8—O3	122.87 (18)
C9—N2—N3	109.45 (15)	O2—C8—C2	125.99 (18)
C10—N3—N2	105.44 (14)	O3—C8—C2	111.14 (15)
C10—N4—N5	118.56 (14)	N2—C9—N4	107.67 (15)
C10—N4—C9	106.04 (15)	N2—C9—C4	128.65 (16)
N5—N4—C9	135.33 (14)	N4—C9—C4	123.68 (15)
C11—N5—N4	107.20 (14)	N3—C10—N4	111.39 (16)
C15—O1—C12	105.97 (15)	N3—C10—S1	139.04 (14)
C8—O3—C16	118.99 (15)	N4—C10—S1	109.55 (13)
C10—S1—C11	87.13 (9)	N5—C11—C12	120.11 (16)
N1—C1—C2	120.65 (16)	N5—C11—S1	117.56 (14)
N1—C1—C7	115.27 (16)	C12—C11—S1	122.33 (13)
C2—C1—C7	124.07 (17)	C13—C12—O1	110.19 (17)
C3—C2—C1	118.28 (17)	C13—C12—C11	133.14 (17)
C3—C2—C8	118.83 (16)	O1—C12—C11	116.66 (15)
C1—C2—C8	122.88 (16)	C12—C13—C14	106.50 (18)
C4—C3—C2	121.00 (16)	C12—C13—H13	126.7
C4—C3—H3	119.5	C14—C13—H13	126.7
C2—C3—H3	119.5	C15—C14—C13	106.87 (18)
C3—C4—C5	117.68 (16)	C15—C14—H14	126.6
C3—C4—C9	119.08 (16)	C13—C14—H14	126.6
C5—C4—C9	123.23 (16)	C14—C15—O1	110.47 (17)
N1—C5—C4	121.21 (16)	C14—C15—H15	124.8
N1—C5—C6	115.29 (16)	O1—C15—H15	124.8

C4—C5—C6	123.50 (16)	O3—C16—C17	109.93 (18)
C5—C6—H6A	109.5	O3—C16—H16A	109.7
C5—C6—H6B	109.5	C17—C16—H16A	109.7
H6A—C6—H6B	109.5	O3—C16—H16B	109.7
C5—C6—H6C	109.5	C17—C16—H16B	109.7
H6A—C6—H6C	109.5	H16A—C16—H16B	108.2
H6B—C6—H6C	109.5	C16—C17—H17A	109.5
C1—C7—H7A	109.5	C16—C17—H17B	109.5
C1—C7—H7B	109.5	H17A—C17—H17B	109.5
H7A—C7—H7B	109.5	C16—C17—H17C	109.5
C1—C7—H7C	109.5	H17A—C17—H17C	109.5
H7A—C7—H7C	109.5	H17B—C17—H17C	109.5
H7B—C7—H7C	109.5		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N5	0.93	2.31	2.982 (3)	128
C13—H13···O2[i]	0.93	2.51	3.285 (3)	141
C17—H17A···O1[ii]	0.96	2.56	3.424 (3)	149

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

Fig. 1

Fig. 2