# Ethyl 4-acetyl-5-anilino-3-methyl-thiophene-2-carboxylate

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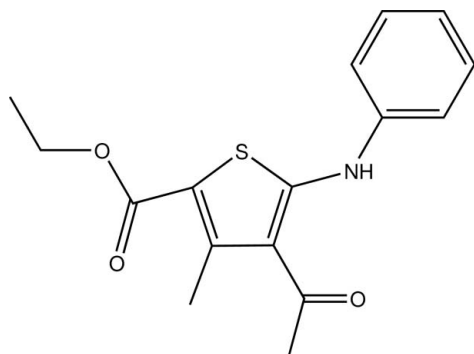Correspondence e-mail: dr.sammer.yousuf@gmail.com

In the title compound, $C_{16}H_{17}NO_3S$, a thiophene derivative with amino phenyl, acetyl, methyl and ethyl carboxyl susbtituents attached to a central thiophene ring, the phenyl and thiophene rings form a dihedral angle of 36.92 (9) Å. The molecular conformation is stabilized by an intramolecular N—H···O hydrogen bond, which forms an $S(6)$ ring motif.

## Related literature

For the biological activity of thiophene derivatives, see: Mishra *et al.* (2011); Mabkhot *et al.* (2013*b*). For the synthesis of fused heterocyclic compounds, see: Sommen *et al.* (2003). For crystal data for related thiophene compounds, see: Mabkhot *et al.* (2013*a,b*); Buehrdel *et al.* (2007).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{16}H_{17}NO_3S$ | $\gamma = 66.785$ (2)° |
| $M_r = 303.37$ | $V = 744.60$ (10) Å$^3$ |
| Triclinic, $P\overline{1}$ | $Z = 2$ |
| $a = 7.9443$ (6) Å | Mo $K\alpha$ radiation |
| $b = 9.5038$ (7) Å | $\mu = 0.23$ mm$^{-1}$ |
| $c = 11.8706$ (9) Å | $T = 273$ K |
| $\alpha = 66.759$ (2)° | $0.45 \times 0.42 \times 0.23$ mm |
| $\beta = 89.754$ (2)° | |

### Data collection

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 10410 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2000) | 3699 independent reflections |
| | 2848 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.905$, $T_{max} = 0.950$ | $R_{int} = 0.028$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.126$ | |
| $S = 1.05$ | |
| 3699 reflections | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 194 parameters | $\Delta\rho_{min} = -0.25$ e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O1 | 0.82 (3) | 1.93 (3) | 2.607 (3) | 140 (2) |

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

## References

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# supporting information

## Ethyl 4-acetyl-5-anilino-3-methylthiophene-2-carboxylate

### Yahia Nasser Mabkhot, Fatima Alatibi, Assem Barakat, M. Iqbal Choudhary and Sammer Yousuf

### S1. Comment

Sulfur containing heterocyclic compounds are well known for their diverse range of biological activities (Mabkhot *et al.*, 2013*b*; Mishra *et al.* 2011). The title compound was synthesized in continuation of our research towards the synthesis of biologically active compounds with fused heterocyclic systems (Mabkhot *et al.*, 2013*b*).

The structure of the title compound (Fig. 1) is composed of a planar thiophene (S1/C2–C5) ring with amino phenyl (N1/C12–C17), acetyl (O1/C10–C11), methyl (C8) and ethyl carboxylate (O2–O3/N2/C6–C7) susbtituents attached to atoms C1, C2,C3 and C4, respectively, of the thiophene ring. The dihedral angle between the planes of thiophene and amino phenyl ring (N1/C11–C16) is 36.92 (9)°. The bond lengths and angles are similar to those of structurally related compounds (Mabkhot *et al.*, 2013*a*,*b*; Buehrdel *et al.*, 2007). The molecular conformation is stabilized by an N1—H1A···O1 intramolecular hydrogen bond (Table 1) to form a *S*6 graph set ring motif. In the crystal packing (Fig. 2), no $\pi \cdots \pi$ or C—H···$\pi$ interactions are observed between adjacent molecules.

### S2. Experimental

The title compound was synthesized by the procedure described in the literature (Sommen *et al.*, 2003). The compound was crystallized by using a mixture of dimethyl formamide and dichloromethane 1:1 *v/v* at room temperature. M. p.: 399 K. Spectral Data: IR (KBr, cm$^{-1}$): 1680, 1700, 2990 cm$^{-1}$; $^1$H-NMR (400 MHz, CDCl$_3$): $\delta$ 1.34 (t, 3H, *J* = 7.1 Hz), 2.58 (s, 3H), 2.82 (s, 3H), 4.28 (q, 2H, *J* = 7.1 Hz), 7.35–7.42 (m, 5H), 12.1 (s, 1H); $^{13}$C-NMR (100 MHz, CDCl$_3$): $\delta$ 14.3, 16.5, 31.3, 60.5, 108.9, 119.2, 120.5, 124.7 (2 C), 129.5 (2 C), 139.6, 145.8, 162.7, 163.4, 195.7; Anal. calcd for C$_{16}$H$_{17}$NO$_3$S: C 63.34; H 5.65; N 4.62. Found: C 63.47; H 5.46; N 4.61.

### S3. Refinement

H atoms on methyl, methylene and methine were positioned geometrically with C—H = 0.96 Å, 0.97 Å and 0.93 Å respectively, and constrained to ride on their parent atoms with $U_{iso}$(H)= 1.2$U_{eq}$ (CH$_2$, CH) and 1.5$U_{eq}$(CH$_3$). The H atoms on the nitrogen atom was located in a difference Fourier map and refined isotropically (N–H= 0.82 (3) Å).
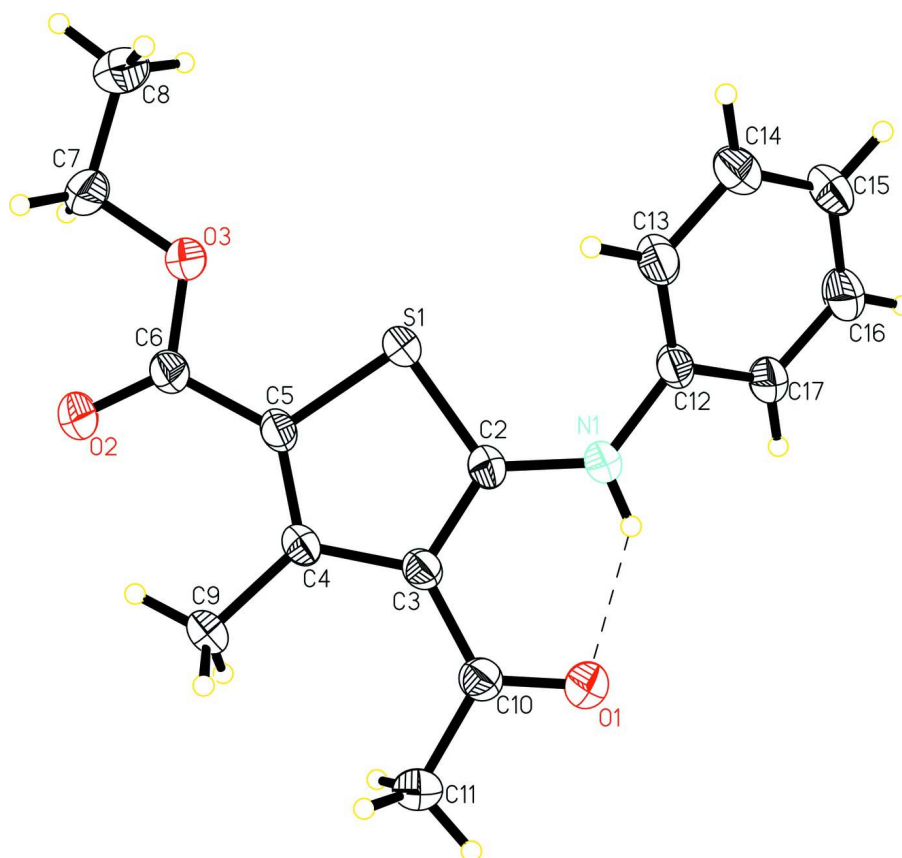
**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.
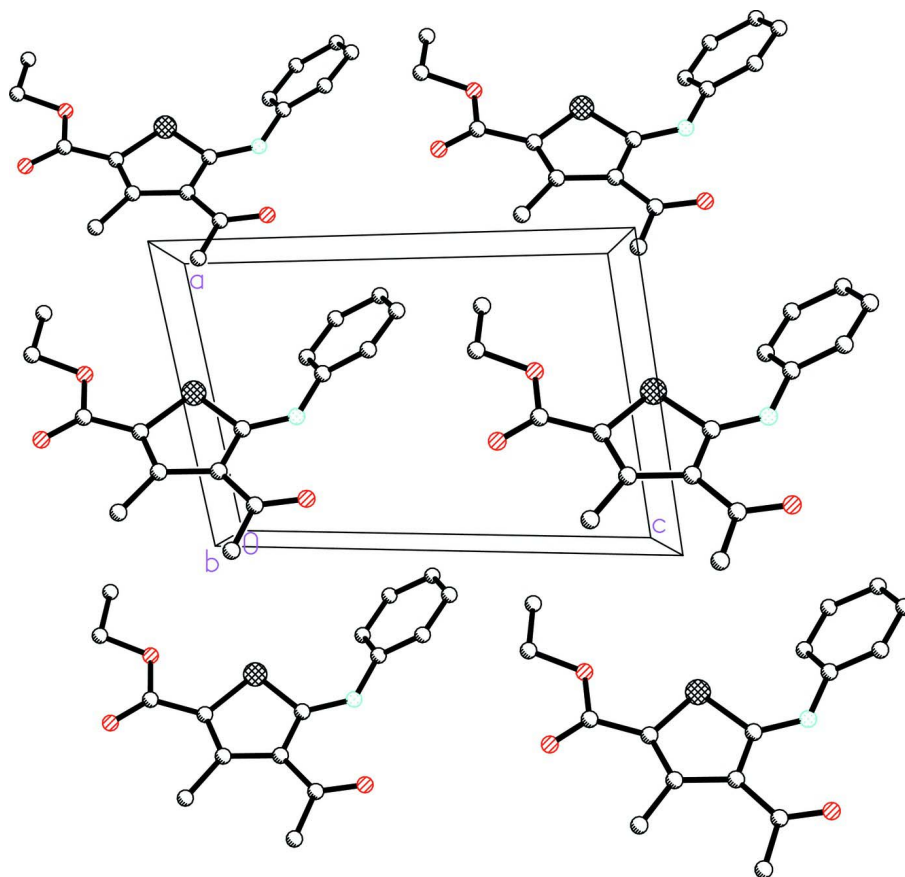
**Figure 2**

Crystal packing of the title compound viewed down the *b* axis. Hydrogen atoms are ommited for clarity.

**Ethyl 4-acetyl-5-anilino-3-methylthiophene-2-carboxylate**

*Crystal data*

| | |
|---|---|
| $C_{16}H_{17}NO_3S$ | $Z = 2$ |
| $M_r = 303.37$ | $F(000) = 320$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.353$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.9443$ (6) Å | Cell parameters from 2619 reflections |
| $b = 9.5038$ (7) Å | $\theta = 2.5$–25.8° |
| $c = 11.8706$ (9) Å | $\mu = 0.23$ mm$^{-1}$ |
| $\alpha = 66.759$ (2)° | $T = 273$ K |
| $\beta = 89.754$ (2)° | Block, yellow |
| $\gamma = 66.785$ (2)° | 0.45 × 0.42 × 0.23 mm |
| $V = 744.60$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | Absorption correction: multi-scan (*SADABS*; Bruker, 2000) |
| Radiation source: fine-focus sealed tube | $T_{min} = 0.905$, $T_{max} = 0.950$ |
| Graphite monochromator | 10410 measured reflections |
| $\omega$ scan | 3699 independent reflections |
| | 2848 reflections with $I > 2\sigma(I)$ |

$R_{int} = 0.028$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 10$

$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.126$ | |
| $S = 1.05$ | H atoms treated by a mixture of independent and constrained refinement |
| 3699 reflections | |
| 194 parameters | $w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.0954P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} < 0.001$ |
| | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.25$ 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.

**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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.48333 (6) | 0.26835 (5) | −0.00730 (4) | 0.04325 (15) |
| O1 | 0.8347 (2) | 0.01329 (18) | −0.22852 (13) | 0.0685 (4) |
| O2 | 0.6413 (2) | −0.06433 (17) | 0.34080 (12) | 0.0704 (5) |
| O3 | 0.41944 (19) | 0.19842 (16) | 0.23323 (11) | 0.0546 (3) |
| N1 | 0.5630 (2) | 0.2832 (2) | −0.23190 (14) | 0.0483 (4) |
| C2 | 0.6046 (2) | 0.1930 (2) | −0.10687 (15) | 0.0404 (4) |
| C3 | 0.7453 (2) | 0.0270 (2) | −0.04358 (15) | 0.0407 (4) |
| C4 | 0.7482 (2) | −0.0370 (2) | 0.08869 (15) | 0.0394 (4) |
| C5 | 0.6149 (2) | 0.0774 (2) | 0.12066 (15) | 0.0419 (4) |
| C6 | 0.5653 (3) | 0.0580 (2) | 0.24344 (16) | 0.0475 (4) |
| C7 | 0.3506 (3) | 0.1937 (3) | 0.34727 (19) | 0.0634 (6) |
| H7A | 0.4503 | 0.1639 | 0.4111 | 0.076* |
| H7B | 0.2996 | 0.1109 | 0.3776 | 0.076* |
| C8 | 0.2028 (3) | 0.3670 (3) | 0.3158 (2) | 0.0728 (6) |
| H8A | 0.1526 | 0.3702 | 0.3889 | 0.109* |
| H8B | 0.1054 | 0.3948 | 0.2524 | 0.109* |
| H8C | 0.2553 | 0.4475 | 0.2858 | 0.109* |
| C9 | 0.8800 (3) | −0.2083 (2) | 0.18489 (17) | 0.0539 (5) |
| H9A | 0.8528 | −0.2197 | 0.2661 | 0.081* |
| H9B | 1.0055 | −0.2205 | 0.1820 | 0.081* |
| H9C | 0.8659 | −0.2944 | 0.1682 | 0.081* |

| | | | |
|---|---|---|---|
| C10 | 0.8559 (2) | −0.0600 (2) | −0.11438 (17) | 0.0466 (4) |
| C11 | 0.9989 (3) | −0.2421 (3) | −0.0534 (2) | 0.0605 (5) |
| H11A | 1.0558 | −0.2749 | −0.1159 | 0.091* |
| H11B | 0.9394 | −0.3133 | −0.0102 | 0.091* |
| H11C | 1.0925 | −0.2538 | 0.0049 | 0.091* |
| C12 | 0.4166 (2) | 0.4428 (2) | −0.30492 (15) | 0.0435 (4) |
| C13 | 0.3570 (3) | 0.5761 (2) | −0.27179 (18) | 0.0536 (5) |
| H13A | 0.4097 | 0.5614 | −0.1958 | 0.064* |
| C14 | 0.2190 (3) | 0.7316 (2) | −0.3516 (2) | 0.0640 (6) |
| H14A | 0.1781 | 0.8210 | −0.3286 | 0.077* |
| C15 | 0.1418 (3) | 0.7551 (3) | −0.4643 (2) | 0.0665 (6) |
| H15A | 0.0501 | 0.8603 | −0.5181 | 0.080* |
| C16 | 0.2008 (3) | 0.6224 (3) | −0.49714 (19) | 0.0653 (6) |
| H16A | 0.1484 | 0.6380 | −0.5735 | 0.078* |
| C17 | 0.3366 (3) | 0.4667 (2) | −0.41818 (17) | 0.0540 (5) |
| H17A | 0.3750 | 0.3772 | −0.4409 | 0.065* |
| H1A | 0.627 (3) | 0.228 (3) | −0.267 (2) | 0.058 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0447 (3) | 0.0347 (2) | 0.0357 (2) | −0.00843 (18) | 0.00177 (18) | −0.00958 (17) |
| O1 | 0.0810 (10) | 0.0576 (9) | 0.0452 (8) | −0.0093 (8) | 0.0116 (7) | −0.0217 (7) |
| O2 | 0.0924 (11) | 0.0462 (8) | 0.0366 (7) | −0.0056 (7) | 0.0057 (7) | −0.0072 (6) |
| O3 | 0.0653 (8) | 0.0428 (7) | 0.0390 (7) | −0.0107 (6) | 0.0109 (6) | −0.0139 (6) |
| N1 | 0.0532 (9) | 0.0401 (8) | 0.0330 (8) | −0.0071 (7) | 0.0017 (7) | −0.0105 (6) |
| C2 | 0.0419 (9) | 0.0394 (9) | 0.0344 (8) | −0.0161 (7) | 0.0013 (7) | −0.0119 (7) |
| C3 | 0.0382 (9) | 0.0379 (8) | 0.0387 (9) | −0.0121 (7) | 0.0011 (7) | −0.0136 (7) |
| C4 | 0.0379 (8) | 0.0348 (8) | 0.0369 (8) | −0.0121 (7) | −0.0019 (7) | −0.0105 (7) |
| C5 | 0.0459 (9) | 0.0357 (8) | 0.0331 (8) | −0.0132 (7) | −0.0013 (7) | −0.0084 (7) |
| C6 | 0.0573 (11) | 0.0370 (9) | 0.0381 (9) | −0.0144 (8) | 0.0025 (8) | −0.0121 (7) |
| C7 | 0.0785 (15) | 0.0569 (12) | 0.0454 (11) | −0.0198 (11) | 0.0207 (10) | −0.0223 (10) |
| C8 | 0.0731 (15) | 0.0667 (14) | 0.0759 (16) | −0.0192 (12) | 0.0235 (13) | −0.0386 (13) |
| C9 | 0.0515 (11) | 0.0418 (10) | 0.0426 (10) | −0.0044 (8) | −0.0029 (8) | −0.0090 (8) |
| C10 | 0.0447 (10) | 0.0452 (10) | 0.0461 (10) | −0.0156 (8) | 0.0045 (8) | −0.0194 (8) |
| C11 | 0.0581 (12) | 0.0510 (11) | 0.0601 (13) | −0.0085 (9) | 0.0104 (10) | −0.0268 (10) |
| C12 | 0.0440 (9) | 0.0390 (9) | 0.0351 (9) | −0.0153 (7) | 0.0041 (7) | −0.0065 (7) |
| C13 | 0.0664 (13) | 0.0430 (10) | 0.0415 (10) | −0.0210 (9) | −0.0020 (9) | −0.0107 (8) |
| C14 | 0.0776 (15) | 0.0396 (10) | 0.0563 (13) | −0.0154 (10) | 0.0040 (11) | −0.0126 (9) |
| C15 | 0.0637 (13) | 0.0466 (11) | 0.0528 (12) | −0.0064 (10) | −0.0046 (10) | −0.0034 (9) |
| C16 | 0.0684 (14) | 0.0613 (13) | 0.0417 (11) | −0.0148 (11) | −0.0086 (10) | −0.0112 (10) |
| C17 | 0.0619 (12) | 0.0493 (10) | 0.0368 (10) | −0.0146 (9) | 0.0011 (8) | −0.0140 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C2 | 1.7182 (18) | C8—H8C | 0.9600 |
| S1—C5 | 1.7422 (16) | C9—H9A | 0.9600 |
| O1—C10 | 1.230 (2) | C9—H9B | 0.9600 |

| | | | |
|---|---|---|---|
| O2—C6 | 1.202 (2) | C9—H9C | 0.9600 |
| O3—C6 | 1.339 (2) | C10—C11 | 1.509 (3) |
| O3—C7 | 1.449 (2) | C11—H11A | 0.9600 |
| N1—C2 | 1.350 (2) | C11—H11B | 0.9600 |
| N1—C12 | 1.409 (2) | C11—H11C | 0.9600 |
| N1—H1A | 0.82 (2) | C12—C13 | 1.379 (3) |
| C2—C3 | 1.409 (2) | C12—C17 | 1.384 (3) |
| C3—C4 | 1.439 (2) | C13—C14 | 1.382 (3) |
| C3—C10 | 1.460 (2) | C13—H13A | 0.9300 |
| C4—C5 | 1.365 (2) | C14—C15 | 1.371 (3) |
| C4—C9 | 1.500 (2) | C14—H14A | 0.9300 |
| C5—C6 | 1.468 (2) | C15—C16 | 1.372 (3) |
| C7—C8 | 1.491 (3) | C15—H15A | 0.9300 |
| C7—H7A | 0.9700 | C16—C17 | 1.374 (3) |
| C7—H7B | 0.9700 | C16—H16A | 0.9300 |
| C8—H8A | 0.9600 | C17—H17A | 0.9300 |
| C8—H8B | 0.9600 | | |
| | | | |
| C2—S1—C5 | 91.06 (8) | C4—C9—H9B | 109.5 |
| C6—O3—C7 | 116.03 (14) | H9A—C9—H9B | 109.5 |
| C2—N1—C12 | 129.39 (17) | C4—C9—H9C | 109.5 |
| C2—N1—H1A | 111.3 (15) | H9A—C9—H9C | 109.5 |
| C12—N1—H1A | 118.8 (15) | H9B—C9—H9C | 109.5 |
| N1—C2—C3 | 124.72 (16) | O1—C10—C3 | 120.70 (17) |
| N1—C2—S1 | 122.77 (13) | O1—C10—C11 | 116.71 (17) |
| C3—C2—S1 | 112.47 (12) | C3—C10—C11 | 122.59 (17) |
| C2—C3—C4 | 111.16 (15) | C10—C11—H11A | 109.5 |
| C2—C3—C10 | 119.78 (15) | C10—C11—H11B | 109.5 |
| C4—C3—C10 | 128.91 (15) | H11A—C11—H11B | 109.5 |
| C5—C4—C3 | 112.44 (14) | C10—C11—H11C | 109.5 |
| C5—C4—C9 | 121.66 (16) | H11A—C11—H11C | 109.5 |
| C3—C4—C9 | 125.89 (16) | H11B—C11—H11C | 109.5 |
| C4—C5—C6 | 129.30 (15) | C13—C12—C17 | 119.32 (16) |
| C4—C5—S1 | 112.85 (13) | C13—C12—N1 | 123.40 (16) |
| C6—C5—S1 | 117.80 (13) | C17—C12—N1 | 117.20 (17) |
| O2—C6—O3 | 123.37 (17) | C12—C13—C14 | 119.95 (18) |
| O2—C6—C5 | 126.39 (17) | C12—C13—H13A | 120.0 |
| O3—C6—C5 | 110.24 (14) | C14—C13—H13A | 120.0 |
| O3—C7—C8 | 106.38 (17) | C15—C14—C13 | 120.5 (2) |
| O3—C7—H7A | 110.5 | C15—C14—H14A | 119.8 |
| C8—C7—H7A | 110.5 | C13—C14—H14A | 119.8 |
| O3—C7—H7B | 110.5 | C14—C15—C16 | 119.61 (19) |
| C8—C7—H7B | 110.5 | C14—C15—H15A | 120.2 |
| H7A—C7—H7B | 108.6 | C16—C15—H15A | 120.2 |
| C7—C8—H8A | 109.5 | C15—C16—C17 | 120.50 (19) |
| C7—C8—H8B | 109.5 | C15—C16—H16A | 119.7 |
| H8A—C8—H8B | 109.5 | C17—C16—H16A | 119.7 |
| C7—C8—H8C | 109.5 | C16—C17—C12 | 120.15 (19) |

| | | | |
|---|---|---|---|
| H8A—C8—H8C | 109.5 | C16—C17—H17A | 119.9 |
| H8B—C8—H8C | 109.5 | C12—C17—H17A | 119.9 |
| C4—C9—H9A | 109.5 | | |

| | | | |
|---|---|---|---|
| C12—N1—C2—C3 | 174.03 (18) | C4—C5—C6—O2 | 3.2 (3) |
| C12—N1—C2—S1 | −3.6 (3) | S1—C5—C6—O2 | −179.74 (17) |
| C5—S1—C2—N1 | 176.62 (16) | C4—C5—C6—O3 | −176.76 (17) |
| C5—S1—C2—C3 | −1.28 (14) | S1—C5—C6—O3 | 0.3 (2) |
| N1—C2—C3—C4 | −176.94 (17) | C6—O3—C7—C8 | 174.54 (18) |
| S1—C2—C3—C4 | 0.91 (19) | C2—C3—C10—O1 | 4.0 (3) |
| N1—C2—C3—C10 | −1.0 (3) | C4—C3—C10—O1 | 179.20 (18) |
| S1—C2—C3—C10 | 176.89 (13) | C2—C3—C10—C11 | −175.38 (17) |
| C2—C3—C4—C5 | 0.1 (2) | C4—C3—C10—C11 | −0.2 (3) |
| C10—C3—C4—C5 | −175.39 (17) | C2—N1—C12—C13 | 39.8 (3) |
| C2—C3—C4—C9 | −179.55 (16) | C2—N1—C12—C17 | −143.5 (2) |
| C10—C3—C4—C9 | 4.9 (3) | C17—C12—C13—C14 | −0.1 (3) |
| C3—C4—C5—C6 | 176.08 (18) | N1—C12—C13—C14 | 176.61 (18) |
| C9—C4—C5—C6 | −4.2 (3) | C12—C13—C14—C15 | −0.7 (3) |
| C3—C4—C5—S1 | −1.09 (19) | C13—C14—C15—C16 | 0.8 (4) |
| C9—C4—C5—S1 | 178.60 (14) | C14—C15—C16—C17 | −0.2 (4) |
| C2—S1—C5—C4 | 1.37 (14) | C15—C16—C17—C12 | −0.6 (3) |
| C2—S1—C5—C6 | −176.16 (15) | C13—C12—C17—C16 | 0.7 (3) |
| C7—O3—C6—O2 | −2.5 (3) | N1—C12—C17—C16 | −176.19 (19) |
| C7—O3—C6—C5 | 177.47 (16) | | |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N1—H1A···O1 | 0.82 (3) | 1.93 (3) | 2.607 (3) | 140 (2) |