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# 1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidin-5-yl]ethanone

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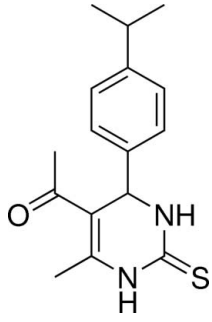
Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.041; $wR$ factor = 0.113; data-to-parameter ratio = 15.8.

In the title molecule, $C_{16}H_{20}N_2OS$, the heterocyclic ring adopts a slightly distorted flattened boat conformation, and the plane through the four coplanar atoms makes a dihedral angle of 86.98 (6)° with the benzene ring. The thione, acetyl and methyl groups lie on the opposite side of the heterocyclic mean plane to the isopropylphenyl group which has an axial orientation. A weak intramolecular C—H···O hydrogen bond is observed. In the crystal, molecules are linked *via* N—H···O, N—H···S and C—H···S hydrogen bonds.

## Related literature

For chemical and biological applications and for the closely related crystal structures of the chloro and fluoro derivatives, see: Anuradha *et al.* (2009, 2012).




## Experimental

### Crystal data

$C_{16}H_{20}N_2OS$
$M_r$ = 288.41
Monoclinic, $C2/c$
$a$ = 26.8413 (5) Å
$b$ = 9.5657 (2) Å
$c$ = 12.0764 (2) Å
$\beta$ = 90.370 (2)°
$V$ = 3100.62 (10) Å$^3$
$Z$ = 8
Cu $K\alpha$ radiation
$\mu$ = 1.83 mm$^{-1}$
$T$ = 123 K
0.49 × 0.23 × 0.18 mm

### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.831, $T_{max}$ = 1.000
5607 measured reflections
3042 independent reflections
2776 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
$S$ = 1.05
3042 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O51$^{i}$ | 0.83 (2) | 2.12 (2) | 2.9445 (17) | 174 (2) |
| N3—H3···S2$^{ii}$ | 0.840 (19) | 2.56 (2) | 3.3481 (13) | 156.9 (18) |
| C61—H61$A$···O51 | 0.98 | 2.22 | 2.9148 (19) | 127 |
| C61—H61$B$···S2$^{iii}$ | 0.98 | 2.86 | 3.7145 (16) | 146 |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2487).

## References

Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Anuradha, N., Thiruvalluvar, A., Chitra, S., Devanathan, D. & Butcher, R. J. (2012). *Acta Cryst.* E**68**, o2625.
Anuradha, N., Thiruvalluvar, A., Pandiarajan, K., Chitra, S. & Butcher, R. J. (2009). *Acta Cryst.* E**65**, o564–o565.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2012). E**68**, o2641 [doi:10.1107/S1600536812034046]

## 1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidin-5-yl]ethanone

**N. Anuradha, A. Thiruvalluvar, S. Chitra, D. Devanathan, Oluwaseun O. Falola and R.J. Butcher**

### S1. Comment

As part of our investigations of dihydropyrimidine derivatives (Anuradha *et al.*, 2009, 2012) to compare their chemical and biological activities, we have undertaken the X-ray crystal structure analysis of the title compound.

In the title molecule, $C_{16}H_{20}N_2OS$ (Fig.1), the heterocyclic ring adopts a slightly distorted flattened boat conformation, and the plane through the four coplanar atoms( C2, N3, C5 and C6) makes a dihedral angle of 86.98 (6)° with the benzene ring. The thione, acetyl and methyl groups have equatorial orientations with respect to the attached heterocyclic ring, whereas the isopropylphenyl group has an axial orientation.

Intermolecular N1—H1···O51, N3—H3···S2 and C61—H61B···S2 hydrogen bonds are found in the crystal structure. A weak intramolecular C61—H61A···O51 hydrogen bond is also observed (Fig. 2, Table 1).

### S2. Experimental

A solution of acetylacetone (1.0012 g, 0.01 mol), 4-isopropylbenzaldehyde (1.48 g, 0.01 mol) and thiourea (1.14 g, 0.015 mol) was heated under reflux in the presence of calcium fluoride (0.07 g, 0.001 mol) for 2 h (monitored by TLC). After completion of the reaction, the reaction mixture was cooled to room temperature and poured into crushed ice. The solid product was filtered under suction and purified by recrystallization from hot methanol to give the product in pure form. Yield 1.86 g (93%).

### S3. Refinement

The two N-bound H atoms were located in a difference Fourier map and refined freely; N1—H1 = 0.83 (2) Å and N3—H3 = 0.840 (19) Å. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C$sp^2$—H = 0.95, *C*(methyl)—H = 0.98, and C(methine)—H = 1.00 Å; $U_{iso}$(H) = k$U_{eq}$(C), where k = 1.5 for methyl H and 1.2 for all other H atoms.

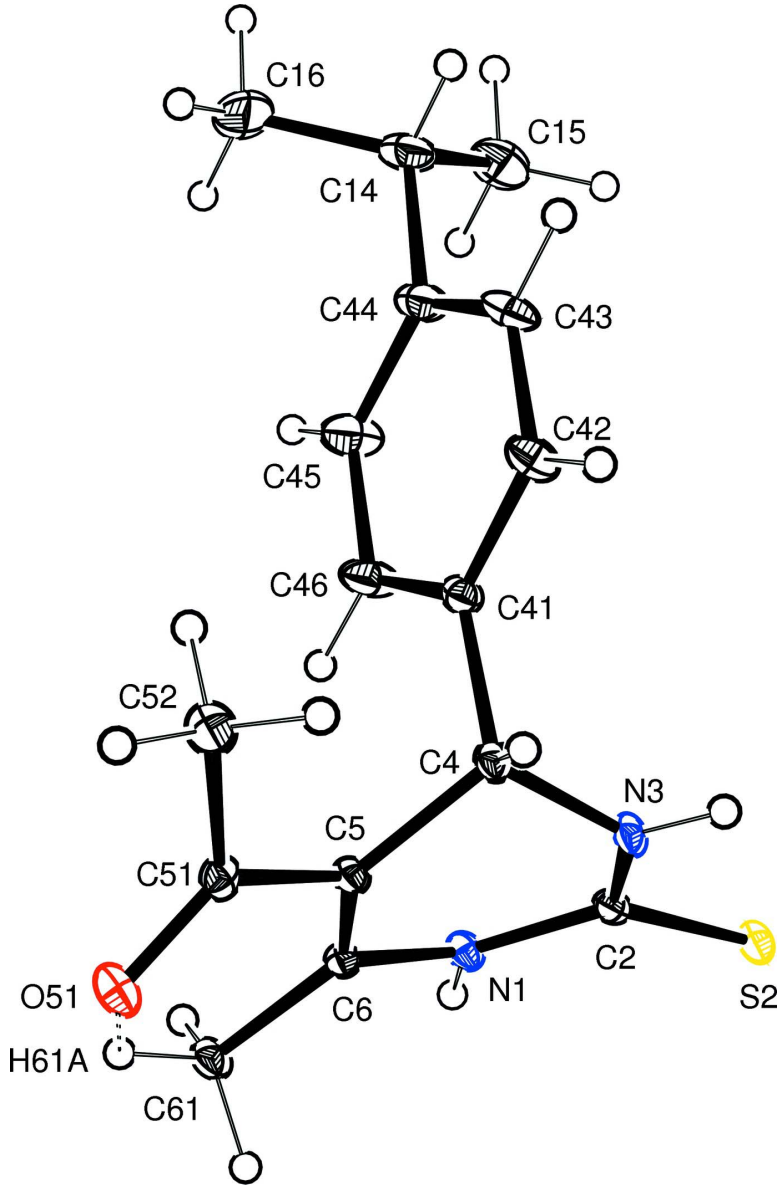


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radius. Dashed lines indicate the intramolecular C—H···O hydrogen bond.

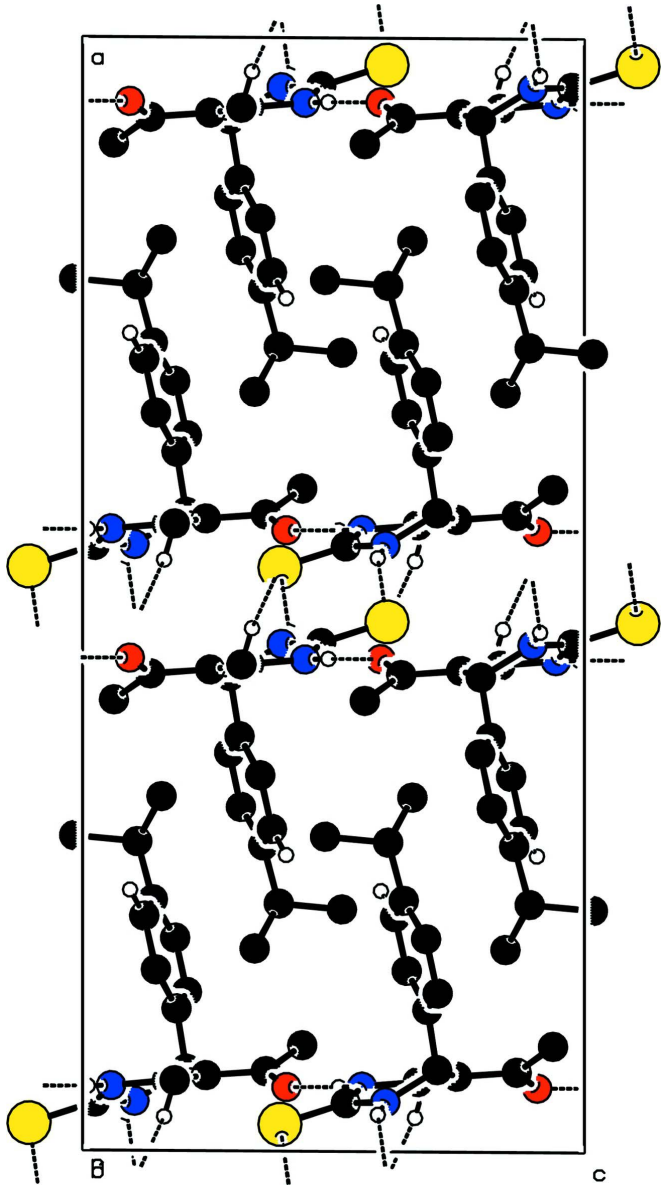


**Figure 2**

The packing of the title compound, viewed down the *b* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

### 1-[4-(4-Isopropylphenyl)-6-methyl-2-sulfanylidene-1,2,3,4- tetrahydropyrimidin-5-yl]ethanone

*Crystal data*

$C_{16}H_{20}N_2OS$
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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 26.8413\ (5)$ Å
$b = 9.5657\ (2)$ Å
$c = 12.0764\ (2)$ Å
$\beta = 90.370\ (2)°$
$V = 3100.62\ (10)$ Å$^3$
$Z = 8$
$F(000) = 1232$
$D_x = 1.236$ Mg m$^{-3}$
Melting point: 486 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 3841 reflections
$\theta = 3.3–73.5°$

$\mu$ = 1.83 mm$^{-1}$
$T$ = 123 K

Prism, colourless
0.49 × 0.23 × 0.18 mm

*Data collection*

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.831, $T_{max}$ = 1.000

5607 measured reflections
3042 independent reflections
2776 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 73.6°, $\theta_{min}$ = 3.3°
$h$ = −30→33
$k$ = −11→10
$l$ = −10→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
$S$ = 1.05
3042 reflections
193 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 1.9078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S2 | 0.02408 (1) | 0.17969 (4) | −0.10663 (3) | 0.0195 (1) |
| O51 | 0.05759 (4) | 0.41789 (12) | 0.40606 (9) | 0.0236 (3) |
| N1 | 0.05834 (5) | 0.34011 (14) | 0.05675 (10) | 0.0163 (3) |
| N3 | 0.04445 (5) | 0.11271 (13) | 0.10324 (10) | 0.0174 (3) |
| C2 | 0.04342 (5) | 0.20984 (16) | 0.02461 (12) | 0.0157 (4) |
| C4 | 0.07362 (5) | 0.12832 (15) | 0.20639 (12) | 0.0163 (4) |
| C5 | 0.06781 (5) | 0.27819 (15) | 0.24566 (12) | 0.0148 (4) |
| C6 | 0.06273 (5) | 0.37919 (15) | 0.16783 (12) | 0.0154 (4) |
| C14 | 0.27761 (7) | −0.0514 (2) | 0.10895 (16) | 0.0335 (6) |
| C15 | 0.28259 (8) | −0.0600 (2) | −0.01678 (18) | 0.0417 (7) |
| C16 | 0.31816 (8) | 0.0428 (3) | 0.1572 (2) | 0.0553 (8) |
| C41 | 0.12759 (6) | 0.08478 (16) | 0.18712 (12) | 0.0184 (4) |
| C42 | 0.14242 (7) | −0.05178 (17) | 0.20769 (14) | 0.0255 (5) |

| | | | | |
|---|---|---|---|---|
| C43 | 0.19116 (7) | −0.09414 (18) | 0.18449 (15) | 0.0294 (5) |
| C44 | 0.22550 (6) | −0.00268 (19) | 0.14005 (14) | 0.0268 (5) |
| C45 | 0.21077 (7) | 0.1352 (2) | 0.12272 (17) | 0.0336 (6) |
| C46 | 0.16255 (7) | 0.17846 (18) | 0.14600 (16) | 0.0295 (5) |
| C51 | 0.07174 (5) | 0.30757 (16) | 0.36521 (12) | 0.0172 (4) |
| C52 | 0.09518 (7) | 0.19628 (17) | 0.43753 (13) | 0.0238 (4) |
| C61 | 0.06312 (6) | 0.53426 (16) | 0.18341 (13) | 0.0205 (4) |
| H1 | 0.0578 (8) | 0.404 (2) | 0.0103 (18) | 0.027 (5)* |
| H3 | 0.0331 (8) | 0.033 (2) | 0.0883 (16) | 0.022 (5)* |
| H4 | 0.05908 | 0.06499 | 0.26360 | 0.0195* |
| H14 | 0.28252 | −0.14749 | 0.13978 | 0.0401* |
| H15A | 0.25674 | −0.12199 | −0.04673 | 0.0625* |
| H15B | 0.31551 | −0.09716 | −0.03547 | 0.0625* |
| H15C | 0.27872 | 0.03349 | −0.04881 | 0.0625* |
| H16A | 0.31439 | 0.13744 | 0.12736 | 0.0829* |
| H16B | 0.35096 | 0.00585 | 0.13732 | 0.0829* |
| H16C | 0.31517 | 0.04545 | 0.23804 | 0.0829* |
| H42 | 0.11939 | −0.11679 | 0.23764 | 0.0305* |
| H43 | 0.20084 | −0.18777 | 0.19963 | 0.0353* |
| H45 | 0.23407 | 0.20068 | 0.09452 | 0.0403* |
| H46 | 0.15335 | 0.27312 | 0.13370 | 0.0353* |
| H52A | 0.09405 | 0.22594 | 0.51515 | 0.0357* |
| H52B | 0.12992 | 0.18230 | 0.41561 | 0.0357* |
| H52C | 0.07678 | 0.10845 | 0.42872 | 0.0357* |
| H61A | 0.07008 | 0.55610 | 0.26127 | 0.0308* |
| H61B | 0.03056 | 0.57263 | 0.16234 | 0.0308* |
| H61C | 0.08898 | 0.57568 | 0.13681 | 0.0308* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S2 | 0.0271 (2) | 0.0143 (2) | 0.0171 (2) | 0.0000 (1) | −0.0027 (1) | −0.0011 (1) |
| O51 | 0.0312 (6) | 0.0183 (6) | 0.0212 (5) | 0.0007 (5) | 0.0029 (4) | −0.0047 (4) |
| N1 | 0.0205 (6) | 0.0117 (6) | 0.0168 (6) | 0.0001 (5) | 0.0005 (5) | 0.0016 (5) |
| N3 | 0.0226 (6) | 0.0101 (6) | 0.0194 (6) | −0.0027 (5) | −0.0022 (5) | −0.0006 (5) |
| C2 | 0.0159 (7) | 0.0132 (7) | 0.0181 (7) | 0.0017 (5) | 0.0011 (5) | −0.0003 (5) |
| C4 | 0.0190 (7) | 0.0129 (7) | 0.0169 (7) | −0.0008 (5) | −0.0005 (5) | 0.0009 (5) |
| C5 | 0.0143 (6) | 0.0123 (7) | 0.0179 (7) | 0.0000 (5) | 0.0005 (5) | −0.0011 (5) |
| C6 | 0.0123 (6) | 0.0145 (7) | 0.0195 (7) | 0.0000 (5) | 0.0009 (5) | −0.0023 (5) |
| C14 | 0.0285 (9) | 0.0315 (10) | 0.0404 (10) | 0.0150 (8) | 0.0036 (7) | −0.0022 (8) |
| C15 | 0.0407 (11) | 0.0405 (12) | 0.0440 (11) | 0.0109 (9) | 0.0115 (9) | −0.0081 (9) |
| C16 | 0.0253 (10) | 0.0666 (16) | 0.0738 (16) | 0.0188 (10) | −0.0064 (10) | −0.0274 (13) |
| C41 | 0.0212 (7) | 0.0157 (7) | 0.0183 (7) | 0.0032 (6) | −0.0008 (5) | −0.0001 (5) |
| C42 | 0.0310 (8) | 0.0164 (8) | 0.0291 (8) | 0.0032 (7) | 0.0035 (6) | 0.0025 (6) |
| C43 | 0.0355 (9) | 0.0177 (8) | 0.0351 (9) | 0.0121 (7) | 0.0026 (7) | 0.0021 (7) |
| C44 | 0.0258 (8) | 0.0260 (9) | 0.0286 (8) | 0.0099 (7) | 0.0008 (6) | −0.0015 (7) |
| C45 | 0.0250 (8) | 0.0262 (10) | 0.0497 (11) | 0.0050 (7) | 0.0091 (7) | 0.0095 (8) |
| C46 | 0.0240 (8) | 0.0187 (9) | 0.0458 (11) | 0.0059 (7) | 0.0065 (7) | 0.0080 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C51 | 0.0154 (7) | 0.0163 (7) | 0.0198 (7) | −0.0041 (5) | 0.0014 (5) | 0.0006 (5) |
| C52 | 0.0312 (8) | 0.0216 (8) | 0.0186 (7) | 0.0011 (7) | −0.0026 (6) | 0.0019 (6) |
| C61 | 0.0268 (8) | 0.0130 (7) | 0.0218 (7) | 0.0025 (6) | −0.0021 (6) | 0.0001 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S2—C2 | 1.6894 (15) | C45—C46 | 1.389 (3) |
| O51—C51 | 1.2262 (19) | C51—C52 | 1.512 (2) |
| N1—C2 | 1.365 (2) | C4—H4 | 1.0000 |
| N1—C6 | 1.3968 (19) | C14—H14 | 1.0000 |
| N3—C2 | 1.3287 (19) | C15—H15A | 0.9800 |
| N3—C4 | 1.4746 (19) | C15—H15B | 0.9800 |
| N1—H1 | 0.83 (2) | C15—H15C | 0.9800 |
| N3—H3 | 0.840 (19) | C16—H16A | 0.9800 |
| C4—C41 | 1.527 (2) | C16—H16B | 0.9800 |
| C4—C5 | 1.518 (2) | C16—H16C | 0.9800 |
| C5—C51 | 1.474 (2) | C42—H42 | 0.9500 |
| C5—C6 | 1.354 (2) | C43—H43 | 0.9500 |
| C6—C61 | 1.495 (2) | C45—H45 | 0.9500 |
| C14—C44 | 1.524 (2) | C46—H46 | 0.9500 |
| C14—C15 | 1.527 (3) | C52—H52A | 0.9800 |
| C14—C16 | 1.526 (3) | C52—H52B | 0.9800 |
| C41—C46 | 1.392 (2) | C52—H52C | 0.9800 |
| C41—C42 | 1.388 (2) | C61—H61A | 0.9800 |
| C42—C43 | 1.400 (3) | C61—H61B | 0.9800 |
| C43—C44 | 1.382 (2) | C61—H61C | 0.9800 |
| C44—C45 | 1.392 (3) | | |
| | | | |
| C2—N1—C6 | 122.71 (13) | C41—C4—H4 | 108.00 |
| C2—N3—C4 | 122.78 (12) | C15—C14—H14 | 108.00 |
| C6—N1—H1 | 117.0 (14) | C16—C14—H14 | 108.00 |
| C2—N1—H1 | 118.5 (14) | C44—C14—H14 | 108.00 |
| C2—N3—H3 | 118.4 (13) | C14—C15—H15A | 109.00 |
| C4—N3—H3 | 117.6 (14) | C14—C15—H15B | 109.00 |
| N1—C2—N3 | 115.51 (13) | C14—C15—H15C | 109.00 |
| S2—C2—N3 | 123.78 (12) | H15A—C15—H15B | 109.00 |
| S2—C2—N1 | 120.71 (11) | H15A—C15—H15C | 109.00 |
| N3—C4—C41 | 110.05 (12) | H15B—C15—H15C | 109.00 |
| C5—C4—C41 | 113.87 (12) | C14—C16—H16A | 109.00 |
| N3—C4—C5 | 107.72 (11) | C14—C16—H16B | 109.00 |
| C4—C5—C6 | 117.84 (13) | C14—C16—H16C | 109.00 |
| C4—C5—C51 | 118.63 (12) | H16A—C16—H16B | 110.00 |
| C6—C5—C51 | 123.37 (13) | H16A—C16—H16C | 109.00 |
| N1—C6—C61 | 112.76 (13) | H16B—C16—H16C | 109.00 |
| C5—C6—C61 | 128.30 (14) | C41—C42—H42 | 120.00 |
| N1—C6—C5 | 118.89 (13) | C43—C42—H42 | 120.00 |
| C15—C14—C16 | 110.16 (17) | C42—C43—H43 | 119.00 |
| C15—C14—C44 | 110.36 (16) | C44—C43—H43 | 119.00 |

| | | | |
|---|---|---|---|
| C16—C14—C44 | 112.27 (16) | C44—C45—H45 | 119.00 |
| C42—C41—C46 | 118.48 (16) | C46—C45—H45 | 120.00 |
| C4—C41—C42 | 120.06 (14) | C41—C46—H46 | 120.00 |
| C4—C41—C46 | 121.43 (14) | C45—C46—H46 | 120.00 |
| C41—C42—C43 | 120.28 (16) | C51—C52—H52A | 109.00 |
| C42—C43—C44 | 121.41 (16) | C51—C52—H52B | 109.00 |
| C14—C44—C43 | 121.18 (16) | C51—C52—H52C | 109.00 |
| C14—C44—C45 | 120.86 (16) | H52A—C52—H52B | 109.00 |
| C43—C44—C45 | 117.95 (16) | H52A—C52—H52C | 109.00 |
| C44—C45—C46 | 121.05 (17) | H52B—C52—H52C | 109.00 |
| C41—C46—C45 | 120.78 (16) | C6—C61—H61A | 109.00 |
| O51—C51—C52 | 120.17 (13) | C6—C61—H61B | 109.00 |
| C5—C51—C52 | 117.29 (13) | C6—C61—H61C | 109.00 |
| O51—C51—C5 | 122.53 (13) | H61A—C61—H61B | 109.00 |
| N3—C4—H4 | 108.00 | H61A—C61—H61C | 109.00 |
| C5—C4—H4 | 108.00 | H61B—C61—H61C | 109.00 |

| | | | |
|---|---|---|---|
| C6—N1—C2—S2 | 163.66 (11) | C51—C5—C6—C61 | 4.0 (2) |
| C6—N1—C2—N3 | −15.1 (2) | C4—C5—C51—O51 | −164.54 (13) |
| C2—N1—C6—C5 | 21.1 (2) | C4—C5—C51—C52 | 16.63 (19) |
| C2—N1—C6—C61 | −161.20 (13) | C6—C5—C51—O51 | 20.2 (2) |
| C4—N3—C2—S2 | 162.66 (11) | C6—C5—C51—C52 | −158.59 (14) |
| C4—N3—C2—N1 | −18.6 (2) | C15—C14—C44—C43 | 107.02 (19) |
| C2—N3—C4—C5 | 41.10 (18) | C15—C14—C44—C45 | −71.9 (2) |
| C2—N3—C4—C41 | −83.58 (17) | C16—C14—C44—C43 | −129.67 (19) |
| N3—C4—C5—C6 | −32.96 (17) | C16—C14—C44—C45 | 51.4 (2) |
| N3—C4—C5—C51 | 151.56 (12) | C4—C41—C42—C43 | 176.53 (15) |
| C41—C4—C5—C6 | 89.38 (16) | C46—C41—C42—C43 | −1.7 (2) |
| C41—C4—C5—C51 | −86.10 (15) | C4—C41—C46—C45 | −176.17 (16) |
| N3—C4—C41—C42 | −92.42 (16) | C42—C41—C46—C45 | 2.0 (3) |
| N3—C4—C41—C46 | 85.75 (17) | C41—C42—C43—C44 | −0.5 (3) |
| C5—C4—C41—C42 | 146.53 (14) | C42—C43—C44—C14 | −176.54 (16) |
| C5—C4—C41—C46 | −35.3 (2) | C42—C43—C44—C45 | 2.4 (3) |
| C4—C5—C6—N1 | 5.98 (19) | C14—C44—C45—C46 | 176.88 (18) |
| C4—C5—C6—C61 | −171.27 (13) | C43—C44—C45—C46 | −2.1 (3) |
| C51—C5—C6—N1 | −178.77 (13) | C44—C45—C46—C41 | −0.2 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O51$^{i}$ | 0.83 (2) | 2.12 (2) | 2.9445 (17) | 174 (2) |
| N3—H3···S2$^{ii}$ | 0.840 (19) | 2.56 (2) | 3.3481 (13) | 156.9 (18) |
| C61—H61*A*···O51 | 0.98 | 2.22 | 2.9148 (19) | 127 |
| C61—H61*B*···S2$^{iii}$ | 0.98 | 2.86 | 3.7145 (16) | 146 |

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