IUCrData

ISSN 2414-3146

Ethyl {[5-acetyl-3-cyano-4-(4-methoxyphenyl)-6-methylpyridin-2-yl]sulfanyl}acetate

Elham A. Al-Taifi,[a]* Manpreet Kaur,[b] Shaaban K. Mohamed,[c,d] Mehmet Akkurt[e] and Jerry P. Jasinski[b]

[a]Department of Chemistry, Faculty of Science, Sana'a University, Sana'a, Yemen, [b]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [c]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [d]Chemistry Department, Faculty of Science, Mini University, 61519 El-Minia, Egypt, and [e]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey. *Correspondence e-mail: shaabankamel@yahoo.com

Received 28 September 2016
Accepted 25 October 2016

Edited by R. J. Butcher, Howard University, USA

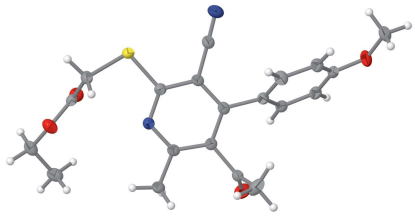
Keywords: crystal structure; pyridine ring; cyano group; hydrogen bonding; ethyl acetate derivative.

CCDC reference: 1511438

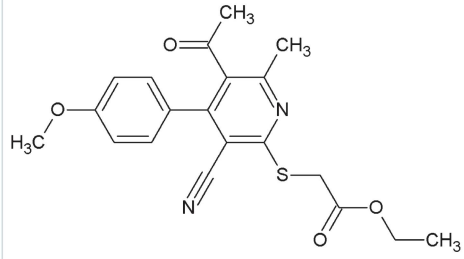
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{20}H_{20}N_2O_4S$, the dihedral angle between the benzene and pyridine rings is 60.97 (7)°. In the crystal, molecules are linked by C—H···O hydrogen bonds and C—H···π interactions, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Pyridine scaffold compounds continue to attract great interest due to their wide variety of interesting biological activities. They exhibit anticancer, analgesic, antimicrobial and antidepressant activities (Kumar *et al.*, 2011). In addition, pyridines are used in the pharmaceutical industry as raw materials for various drugs, vitamins and fungicides (Kumar *et al.*, 2011). These facts promoted us to synthesize and determine the crystal structure of the title compound.

The dihedral angle between the benzene and pyridine rings of the title molecule (Fig. 1) is 60.97 (7)°. The torsion C10—C11—O4—C20, C5—C6—C15—C16, C5—C6—C15—O3, N1—C3—S1—C2, C3—S1—C2—C1, C2—C1—O2—C18 and C1—O2—C18—C19 are 3.6 (2), 73.37 (19), −109.33 (17), −20.05 (13), −73.89 (12), −174.92 (13) and 75.85 (18), respectively. All bonds and bond angles in the title molecule are within the normal range.

In the crystal structure, adjacent molecules are connected *via* C—H···O hydrogen bonds and C—H···π interactions with each to other, forming a three-dimensional network (Fig. 2 and Table 1).

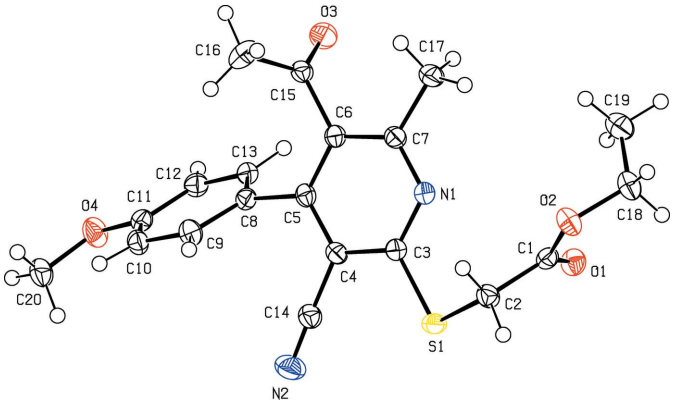


Figure 1
The title molecule shown with 50% probability displacement ellipsoids.

Synthesis and crystallization

To a mixture of 5-acetyl-3-cyano-4-(4-methoxyphenyl)-6-methylpyridine-2(1*H*)-thione (10 mmol) and ethyl chloroacetate (10 mmol) in ethanol (20 ml), sodium acetate trihydrate (11 mmol) was added. The resulting mixture was heated under reflux for 2 h and then allowed to cool. The precipitated solid was collected and recrystallized from ethanol (yield 98%; m.p. 409–410 K). IR: 2200 (CN), 1730 (C═O, ester), 1690 (C═O, acetyl) cm^{-1}. ^{1}H NMR ($CDCl_3$): 6.9–7.4 (*dd*, 4H, ArH); 4.1–4.3 (*q*, 2H, OCH_2); 3.9 (*s*, 2H, SCH_2); 3.7 (*s*, 3H, OCH_3); 2.4 (*s*, 3H, $COCH_3$); 1.8 (*s*, 3H, CH_3 at C-6); 1.1–1.3 (*t*, 3H, CH_3 of ester).

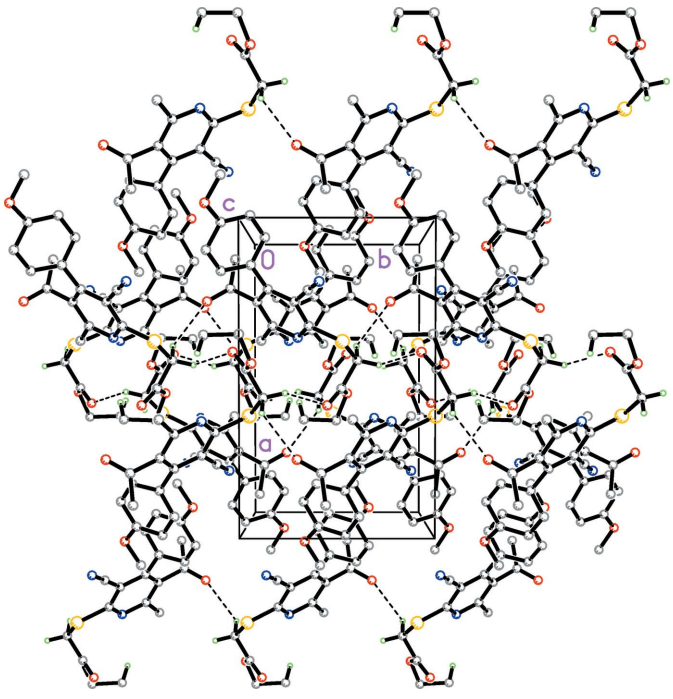


Figure 2
Packing of the title molecule viewed down the *c* axis with the hydrogen bonds shown by dotted lines.

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

*Cg*1 and *Cg*2 are the centroids of the pyridine (N1/C3–C7) and benzene (C8–C13) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O3^{i}	0.99	2.52	3.150 (2)	121
C2—H2*B*···O1^{ii}	0.99	2.52	3.3345 (19)	140
C19—H19*C*···O2^{iii}	0.98	2.65	3.437 (2)	138
C9—H9···*Cg*2^{iv}	0.95	2.88	3.7803 (17)	159
C20—H20*B*···*Cg*1^{v}	0.98	2.84	3.5619 (18)	131

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, -y+2, -z+2$; (iv) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{20}N_2O_4S$
M_r	384.44
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	13.4883 (2), 8.23273 (16), 16.8923 (3)
β (°)	93.8000 (17)
V (Å^3)	1871.69 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.78
Crystal size (mm)	0.49 × 0.46 × 0.22
Data collection	
Diffractometer	Rigaku Oxford Diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.600, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6913, 3553, 3278
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.112, 1.05
No. of reflections	3553
No. of parameters	249
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.29

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

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

Acknowledgements

JPJ would like to acknowledge the NSF–MRI program (grant No. CHE-1039027) for funds to purchase the *X* ray diffractometer.

References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Kumar, S., Sharma, P. K., Dudhe, R. & Kumar, N. (2011). *J. Chronother. Drug Deliv*, **2**, 71–78.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x161715 [https://doi.org/10.1107/S2414314616017156]

Ethyl {[5-acetyl-3-cyano-4-(4-methoxyphenyl)-6-methylpyridin-2-yl]sulfanyl}acetate

Elham A. Al-Taifi, Manpreet Kaur, Shaaban K. Mohamed, Mehmet Akkurt and Jerry P. Jasinski

Ethyl {[5-acetyl-3-cyano-4-(4-methoxyphenyl)-6-methylpyridin-2-yl]sulfanyl}acetate

Crystal data

$C_{20}H_{20}N_2O_4S$
M_r = 384.44
Monoclinic, $P2_1/c$
a = 13.4883 (2) Å
b = 8.23273 (16) Å
c = 16.8923 (3) Å
β = 93.8000 (17)°
V = 1871.69 (6) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.364 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3634 reflections
θ = 4.1–71.5°
μ = 1.78 mm^{-1}
T = 173 K
Irregular, colourless
0.49 × 0.46 × 0.22 mm

Data collection

Rigaku Oxford Diffraction diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.600, T_{max} = 1.000
6913 measured reflections
3553 independent reflections
3278 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 71.2°, θ_{min} = 3.3°
h = −16→15
k = −9→6
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.05
3553 reflections
249 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0702P)^2 + 0.4141P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0045 (4)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.62202 (3)	1.02799 (5)	0.73252 (2)	0.02850 (15)
O1	0.41273 (8)	0.94698 (14)	0.79041 (6)	0.0281 (3)
O2	0.45128 (8)	1.05466 (14)	0.91107 (6)	0.0282 (3)
O3	0.75861 (9)	0.29044 (14)	0.87453 (8)	0.0367 (3)
O4	1.05277 (9)	0.32068 (14)	0.56752 (7)	0.0331 (3)
N1	0.63715 (9)	0.78612 (15)	0.83887 (7)	0.0222 (3)
N2	0.80930 (12)	0.90691 (19)	0.60820 (9)	0.0378 (4)
C1	0.46752 (11)	1.02342 (17)	0.83507 (9)	0.0222 (3)
C2	0.56182 (11)	1.10919 (18)	0.81526 (9)	0.0248 (3)
H2A	0.6093	1.1056	0.8625	0.030*
H2B	0.5460	1.2247	0.8043	0.030*
C3	0.67375 (10)	0.84809 (18)	0.77408 (8)	0.0212 (3)
C4	0.75159 (10)	0.77387 (18)	0.73602 (8)	0.0208 (3)
C5	0.79313 (10)	0.62958 (18)	0.76679 (8)	0.0204 (3)
C6	0.75585 (10)	0.56783 (18)	0.83602 (8)	0.0207 (3)
C7	0.67650 (10)	0.64734 (18)	0.86890 (8)	0.0217 (3)
C8	0.86906 (11)	0.54322 (18)	0.72251 (8)	0.0208 (3)
C9	0.95693 (11)	0.61926 (19)	0.70468 (9)	0.0254 (3)
H9	0.9722	0.7235	0.7262	0.030*
C10	1.02267 (11)	0.54571 (19)	0.65599 (9)	0.0243 (3)
H10	1.0839	0.5966	0.6463	0.029*
C11	0.99780 (11)	0.39687 (18)	0.62161 (9)	0.0231 (3)
C12	0.91130 (11)	0.31666 (18)	0.64035 (9)	0.0245 (3)
H12	0.8958	0.2131	0.6180	0.029*
C13	0.84814 (10)	0.38804 (18)	0.69154 (9)	0.0221 (3)
H13	0.7905	0.3317	0.7057	0.027*
C14	0.78475 (11)	0.84630 (19)	0.66472 (9)	0.0254 (3)
C15	0.80209 (11)	0.41777 (18)	0.87574 (8)	0.0221 (3)
C16	0.90163 (13)	0.4406 (2)	0.91893 (11)	0.0347 (4)
H16A	0.8959	0.5187	0.9622	0.052*
H16B	0.9488	0.4817	0.8821	0.052*
H16C	0.9253	0.3363	0.9408	0.052*
C17	0.62897 (13)	0.5812 (2)	0.94013 (10)	0.0302 (4)
H17A	0.5897	0.6668	0.9635	0.045*
H17B	0.6807	0.5437	0.9794	0.045*
H17C	0.5855	0.4901	0.9240	0.045*
C18	0.35925 (12)	0.9943 (2)	0.94011 (10)	0.0300 (4)
H18A	0.3038	1.0188	0.9006	0.036*
H18B	0.3462	1.0517	0.9899	0.036*

C19	0.36222 (13)	0.8147 (2)	0.95549 (10)	0.0340 (4)
H19A	0.3677	0.7566	0.9053	0.051*
H19B	0.3012	0.7813	0.9794	0.051*
H19C	0.4197	0.7888	0.9918	0.051*
C20	1.13748 (12)	0.4044 (2)	0.54211 (10)	0.0327 (4)
H20A	1.1696	0.3381	0.5030	0.049*
H20B	1.1845	0.4244	0.5878	0.049*
H20C	1.1166	0.5083	0.5180	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0316 (2)	0.0278 (2)	0.0272 (2)	0.00865 (15)	0.01043 (16)	0.00996 (14)
O1	0.0252 (5)	0.0322 (6)	0.0262 (6)	−0.0021 (5)	−0.0026 (4)	−0.0026 (4)
O2	0.0259 (5)	0.0345 (6)	0.0248 (6)	−0.0081 (5)	0.0054 (4)	−0.0048 (4)
O3	0.0307 (6)	0.0269 (6)	0.0525 (7)	−0.0050 (5)	0.0021 (5)	0.0100 (5)
O4	0.0322 (6)	0.0278 (6)	0.0413 (6)	0.0027 (5)	0.0161 (5)	−0.0049 (5)
N1	0.0195 (6)	0.0241 (6)	0.0234 (6)	0.0019 (5)	0.0037 (5)	0.0025 (5)
N2	0.0459 (9)	0.0391 (8)	0.0298 (7)	0.0026 (7)	0.0132 (6)	0.0077 (6)
C1	0.0222 (7)	0.0207 (7)	0.0235 (7)	0.0042 (6)	0.0010 (6)	0.0022 (6)
C2	0.0251 (7)	0.0211 (7)	0.0288 (7)	0.0009 (6)	0.0075 (6)	0.0008 (6)
C3	0.0189 (7)	0.0226 (7)	0.0221 (7)	−0.0005 (5)	0.0012 (5)	0.0018 (5)
C4	0.0202 (6)	0.0230 (7)	0.0195 (6)	−0.0021 (5)	0.0029 (5)	0.0005 (5)
C5	0.0172 (6)	0.0230 (7)	0.0208 (6)	−0.0024 (5)	0.0008 (5)	−0.0020 (6)
C6	0.0186 (7)	0.0214 (7)	0.0219 (7)	−0.0016 (5)	0.0000 (5)	0.0001 (6)
C7	0.0206 (7)	0.0237 (7)	0.0207 (7)	−0.0020 (6)	0.0016 (5)	0.0011 (6)
C8	0.0186 (7)	0.0236 (7)	0.0201 (7)	0.0016 (5)	0.0004 (5)	0.0010 (5)
C9	0.0233 (7)	0.0258 (8)	0.0270 (7)	−0.0044 (6)	0.0018 (6)	−0.0041 (6)
C10	0.0189 (7)	0.0262 (8)	0.0279 (7)	−0.0019 (6)	0.0030 (6)	0.0001 (6)
C11	0.0228 (7)	0.0228 (7)	0.0240 (7)	0.0053 (6)	0.0035 (6)	0.0026 (6)
C12	0.0250 (7)	0.0200 (7)	0.0285 (7)	0.0001 (6)	0.0019 (6)	0.0000 (6)
C13	0.0188 (7)	0.0225 (7)	0.0250 (7)	−0.0003 (5)	0.0014 (5)	0.0029 (6)
C14	0.0252 (7)	0.0260 (8)	0.0254 (8)	0.0011 (6)	0.0051 (6)	0.0003 (6)
C15	0.0236 (7)	0.0219 (7)	0.0214 (7)	0.0020 (6)	0.0058 (5)	0.0010 (6)
C16	0.0357 (9)	0.0247 (8)	0.0416 (10)	0.0044 (7)	−0.0126 (7)	−0.0005 (7)
C17	0.0317 (8)	0.0309 (8)	0.0291 (8)	0.0052 (7)	0.0115 (6)	0.0082 (7)
C18	0.0246 (8)	0.0367 (9)	0.0294 (8)	−0.0035 (7)	0.0077 (6)	−0.0032 (7)
C19	0.0348 (8)	0.0386 (9)	0.0292 (8)	−0.0068 (7)	0.0055 (7)	0.0022 (7)
C20	0.0278 (8)	0.0364 (9)	0.0352 (8)	0.0043 (7)	0.0127 (7)	0.0006 (7)

Geometric parameters (Å, º)

S1—C2	1.7917 (15)	C9—H9	0.9500
S1—C3	1.7630 (15)	C9—C10	1.388 (2)
O1—C1	1.1988 (19)	C10—H10	0.9500
O2—C1	1.3415 (18)	C10—C11	1.388 (2)
O2—C18	1.4522 (19)	C11—C12	1.395 (2)
O3—C15	1.201 (2)	C12—H12	0.9500

O4—C11	1.3666 (18)	C12—C13	1.384 (2)
O4—C20	1.425 (2)	C13—H13	0.9500
N1—C3	1.3318 (18)	C15—C16	1.497 (2)
N1—C7	1.345 (2)	C16—H16A	0.9800
N2—C14	1.145 (2)	C16—H16B	0.9800
C1—C2	1.512 (2)	C16—H16C	0.9800
C2—H2A	0.9900	C17—H17A	0.9800
C2—H2B	0.9900	C17—H17B	0.9800
C3—C4	1.407 (2)	C17—H17C	0.9800
C4—C5	1.399 (2)	C18—H18A	0.9900
C4—C14	1.441 (2)	C18—H18B	0.9900
C5—C6	1.399 (2)	C18—C19	1.502 (2)
C5—C8	1.489 (2)	C19—H19A	0.9800
C6—C7	1.400 (2)	C19—H19B	0.9800
C6—C15	1.520 (2)	C19—H19C	0.9800
C7—C17	1.502 (2)	C20—H20A	0.9800
C8—C9	1.391 (2)	C20—H20B	0.9800
C8—C13	1.402 (2)	C20—H20C	0.9800

C3—S1—C2	100.99 (7)	C11—C12—H12	120.0
C1—O2—C18	117.07 (12)	C13—C12—C11	119.96 (14)
C11—O4—C20	117.44 (13)	C13—C12—H12	120.0
C3—N1—C7	118.48 (12)	C8—C13—H13	119.9
O1—C1—O2	124.74 (14)	C12—C13—C8	120.19 (13)
O1—C1—C2	126.77 (14)	C12—C13—H13	119.9
O2—C1—C2	108.39 (12)	N2—C14—C4	178.24 (17)
S1—C2—H2A	108.4	O3—C15—C6	121.09 (13)
S1—C2—H2B	108.4	O3—C15—C16	122.63 (14)
C1—C2—S1	115.46 (11)	C16—C15—C6	116.22 (13)
C1—C2—H2A	108.4	C15—C16—H16A	109.5
C1—C2—H2B	108.4	C15—C16—H16B	109.5
H2A—C2—H2B	107.5	C15—C16—H16C	109.5
N1—C3—S1	119.38 (11)	H16A—C16—H16B	109.5
N1—C3—C4	122.54 (13)	H16A—C16—H16C	109.5
C4—C3—S1	118.07 (11)	H16B—C16—H16C	109.5
C3—C4—C14	118.99 (13)	C7—C17—H17A	109.5
C5—C4—C3	119.46 (13)	C7—C17—H17B	109.5
C5—C4—C14	121.53 (13)	C7—C17—H17C	109.5
C4—C5—C6	117.52 (13)	H17A—C17—H17B	109.5
C4—C5—C8	119.40 (12)	H17A—C17—H17C	109.5
C6—C5—C8	122.95 (13)	H17B—C17—H17C	109.5
C5—C6—C7	119.22 (13)	O2—C18—H18A	109.1
C5—C6—C15	120.31 (13)	O2—C18—H18B	109.1
C7—C6—C15	120.46 (13)	O2—C18—C19	112.44 (14)
N1—C7—C6	122.72 (13)	H18A—C18—H18B	107.8
N1—C7—C17	115.53 (13)	C19—C18—H18A	109.1
C6—C7—C17	121.75 (13)	C19—C18—H18B	109.1
C9—C8—C5	121.23 (13)	C18—C19—H19A	109.5

C9—C8—C13	118.85 (13)	C18—C19—H19B	109.5
C13—C8—C5	119.64 (13)	C18—C19—H19C	109.5
C8—C9—H9	119.4	H19A—C19—H19B	109.5
C10—C9—C8	121.27 (14)	H19A—C19—H19C	109.5
C10—C9—H9	119.4	H19B—C19—H19C	109.5
C9—C10—H10	120.4	O4—C20—H20A	109.5
C11—C10—C9	119.14 (14)	O4—C20—H20B	109.5
C11—C10—H10	120.4	O4—C20—H20C	109.5
O4—C11—C10	123.93 (13)	H20A—C20—H20B	109.5
O4—C11—C12	115.68 (14)	H20A—C20—H20C	109.5
C10—C11—C12	120.37 (14)	H20B—C20—H20C	109.5
S1—C3—C4—C5	−178.97 (11)	C5—C8—C13—C12	170.24 (13)
S1—C3—C4—C14	−0.71 (19)	C6—C5—C8—C9	−125.95 (16)
O1—C1—C2—S1	−25.7 (2)	C6—C5—C8—C13	60.16 (19)
O2—C1—C2—S1	157.87 (10)	C7—N1—C3—S1	178.89 (10)
O4—C11—C12—C13	−176.80 (13)	C7—N1—C3—C4	0.1 (2)
N1—C3—C4—C5	−0.2 (2)	C7—C6—C15—O3	71.7 (2)
N1—C3—C4—C14	178.08 (13)	C7—C6—C15—C16	−105.64 (17)
C1—O2—C18—C19	75.85 (18)	C8—C5—C6—C7	−172.72 (13)
C2—S1—C3—N1	20.05 (13)	C8—C5—C6—C15	8.3 (2)
C2—S1—C3—C4	−161.11 (12)	C8—C9—C10—C11	3.0 (2)
C3—S1—C2—C1	−73.89 (12)	C9—C8—C13—C12	−3.8 (2)
C3—N1—C7—C6	1.6 (2)	C9—C10—C11—O4	174.13 (14)
C3—N1—C7—C17	−177.76 (13)	C9—C10—C11—C12	−4.7 (2)
C3—C4—C5—C6	−1.4 (2)	C10—C11—C12—C13	2.1 (2)
C3—C4—C5—C8	174.50 (13)	C11—C12—C13—C8	2.2 (2)
C4—C5—C6—C7	3.1 (2)	C13—C8—C9—C10	1.2 (2)
C4—C5—C6—C15	−175.95 (12)	C14—C4—C5—C6	−179.65 (13)
C4—C5—C8—C9	58.34 (19)	C14—C4—C5—C8	−3.7 (2)
C4—C5—C8—C13	−115.55 (16)	C15—C6—C7—N1	175.72 (13)
C5—C6—C7—N1	−3.3 (2)	C15—C6—C7—C17	−4.9 (2)
C5—C6—C7—C17	176.07 (14)	C18—O2—C1—O1	−1.6 (2)
C5—C6—C15—O3	−109.33 (17)	C18—O2—C1—C2	174.92 (13)
C5—C6—C15—C16	73.37 (19)	C20—O4—C11—C10	−3.6 (2)
C5—C8—C9—C10	−172.76 (14)	C20—O4—C11—C12	175.24 (13)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the pyridine (N1/C3–C7) and benzene (C8–C13) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O3^{i}	0.99	2.52	3.150 (2)	121
C2—H2*B*···O1^{ii}	0.99	2.52	3.3345 (19)	140
C19—H19*C*···O2^{iii}	0.98	2.65	3.437 (2)	138
C9—H9···*Cg*2^{iv}	0.95	2.88	3.7803 (17)	159
C20—H20*B*···*Cg*1^{v}	0.98	2.84	3.5619 (18)	131

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, *y*+1/2, −*z*+3/2; (iii) −*x*+1, −*y*+2, −*z*+2; (iv) −*x*+2, *y*+1/2, −*z*+3/2; (v) −*x*+2, *y*−1/2, −*z*+3/2.