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(*E*)-2-Phenyl-*N*-(thiophen-2-ylmethylidene)-imidazo[1,2-*a*]pyridin-3-amine

Abdelmalik Elaatiaoui,[a]* Fouad Elkalai,[a] Noureddine Benchat,[a] Mohamed Saadi[b] and Lahcen El Ammari[b]

[a]Laboratoire de Chimie Appliquée et Environnement (LCAE), Faculté des Sciences, Université Mohammed Premier, BP 524, 60000 Oujda, Morocco, and [b]Laboratoire de Chimie du Solide Appliquée, Faculty of Sciences, Mohammed V University in Rabat, Avenue Ibn Battouta, BP 1014, Rabat, Morocco. *Correspondence e-mail: a_elaatiaoui@yahoo.fr

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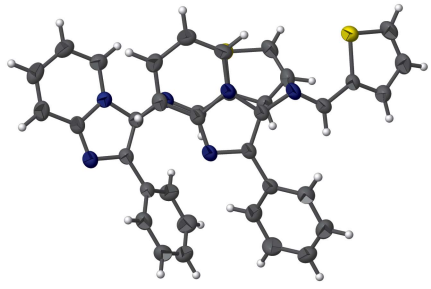
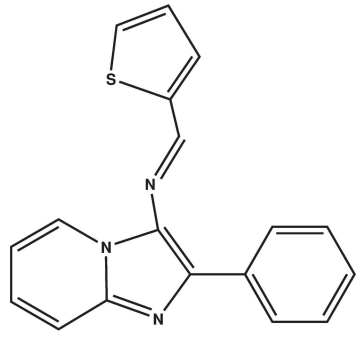
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{18}H_{13}N_3S$, is build up from two independent molecules slightly inclined to each other. In each molecule, the imidazo[1,2-*a*]pyridine ring system is almost planar, with the largest deviation from the mean plane being 0.022 (1) Å in the first molecule and 0.018 (1) Å in the second molecule. The fused-ring system belonging to the first molecule makes dihedral angles of 24.06 (7) and 40.52 (8)° with the thiophenyl and phenyl rings, respectively. The corresponding values observed in the second molecule are nearly the same, namely 25.20 (7) and 38.99 (7)°, respectively. The dihedral angle between the thiophenyl and phenyl rings is 63.47 (9)° in the first molecule and 47.49 (9)° in the second. The cohesion of the crystal structure is ensured by two C—H$\cdots$N hydrogen bonds between molecules and by three C—H$\cdots\pi$ interactions, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Schiff bases bearing an azomethine functional group –C=N–, have gained importance in the pharmaceutical and medicinal industries due to their widespread potential biological activities such as anticancer (Ren *et al.*, 2002), antibacterial and antifungal activities (Shi *et al.*, 2007), anticonvulsant (Sridhar *et al.*, 2002; Kaplan *et al.*, 1980), antituberculosis (Patole *et al.*, 2006; Hearn & Cynamon, 2004), analgesic and anti-inflammatory properties (Bhandari *et al.*, 2008). The present paper is a continuation of our research work devoted to the development of imidazo[1,2-*a*]pyridine derivatives with potential pharmacological activities (Elaatiaoui *et al.*, 2014, 2015).

The heterobicyclic ring system in the title compound is essentially planar, with a maximum deviation of 0.022 (1) Å for atom C6 in the first molecule (S1/N1–N3/C1–C18)

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

*Cg*1 and *Cg*2 are the centroids of the C31–C36 and C13–C18 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···N3^{i}	0.93	2.50	3.428 (2)	175
C14—H14···N6^{ii}	0.93	2.61	3.526 (2)	170
C15—H15···*Cg*1^{ii}	0.93	2.97	3.778 (2)	146
C18—H18···*Cg*1	0.93	2.88	3.761 (2)	157
C33—H33···*Cg*2^{iii}	0.93	2.95	3.814 (2)	155

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

and 0.018 (1) Å for atom N5 in the second molecule (S2/N4–N6/C19–C36) (Fig. 1). In the first molecule, the dihedral angles between the mean plane through the fused-ring system (N2/N3/C6–C12) and the thiophen-2-yl (S1/C1–C4) and phenyl (C13–C18) rings are of 24.06 (7) and 40.52 (8)°, respectively. Nearly the same values are observed in the second molecule between the imidazo[1,2-*a*]pyridin system and the thiophen-2-

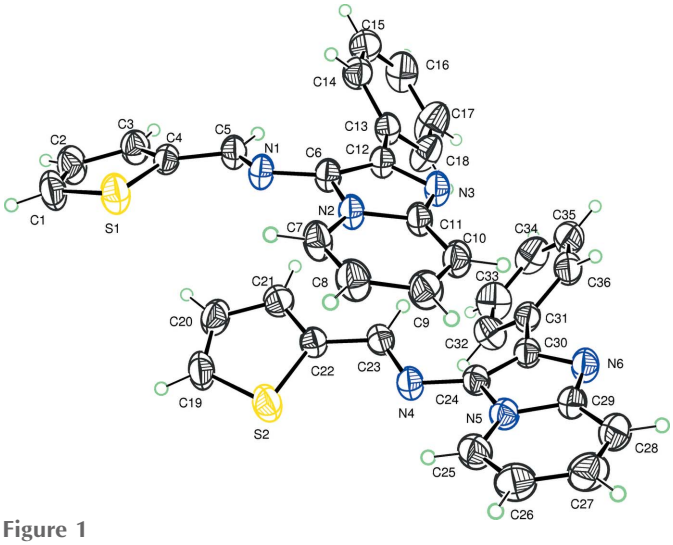


Figure 1
Plot of the molecule of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

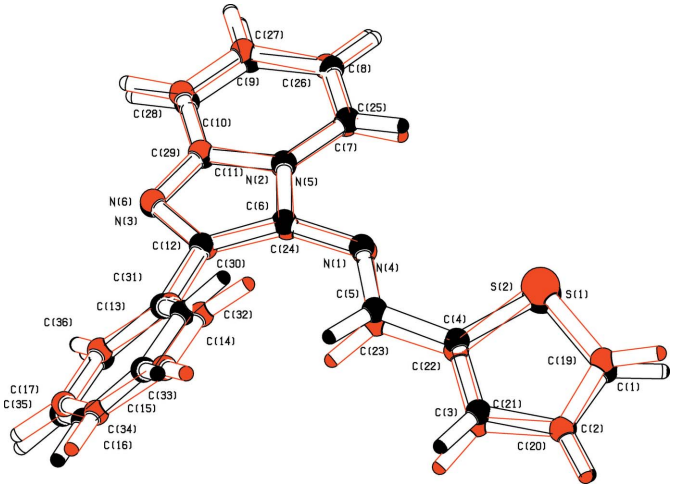


Figure 2
Least-squares fit of the two molecules in the asymmetric unit (one molecule inverted); the r.m.s. deviation for all non-H atoms is 0.263 Å.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{13}N_3S$
M_r	303.37
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	9.6524 (17), 10.1168 (17), 16.655 (3)
α, β, γ (°)	101.299 (8), 106.315 (9), 95.628 (8)
V (Å^3)	1510.3 (5)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.21
Crystal size (mm)	0.44 × 0.21 × 0.12
Data collection	
Diffractometer	Bruker X8 *APEX*
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.641, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	66495, 8471, 5839
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.694
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.125, 1.02
No. of reflections	8471
No. of parameters	397
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

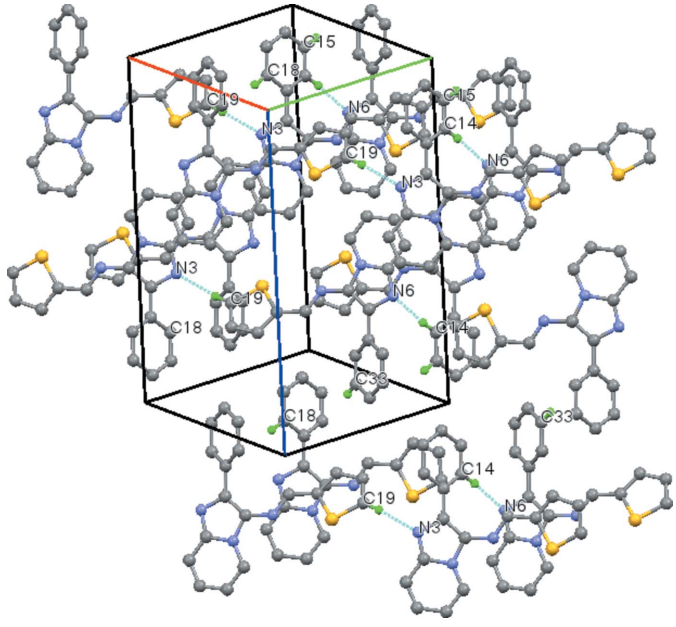


Figure 3
Three-dimensional plot of the title compound showing molecules linked by hydrogen bonds (dashed blue lines) and C—H···π interactions (dashed green lines).

yl (S2/C19–C22) and the phenyl (C31–C36) rings, *viz*. 25.20 (7) and 38.99 (7)°, respectively. The dihedral angle between the thiophen-2-yl and phenyl rings is 63.47 (9)° in the first molecule and 47.49 (9)° in the second. A least-squares fit of the two molecules is shown in Fig. 2.

In the crystal, molecules are linked together by two C—H···N hydrogen bonds between the molecules and by C—H···π interactions, forming a three dimensional network (Fig. 3 and Table 1).

Synthesis and crystallization

A solution of 2-phenylimidazo[1,2-*a*]pyridin-3-amine (0.5 g, 2.39 mmol) and thiophene-2-carbaldehyde (0.27 g, 2.39 mmol) in 20 ml of dry diethyl ether was stirred at room temperature for 24 h using a 0.3 ml of acetic acid as catalyst. The solvent was evaporated. The resulting solid purified by column chromatography (CH_2Cl_2/MeOH 99/1) and crystallized from methanol to give the final yellow product (yield 86.15%, m.p. = 399 K).

Spectroscopic data: (*E*)-*N*-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-(thiophen-2-yl)methanimine. R_f = 0.55 (silica, CH_2Cl_2/MeOH, 9/1). ^{1}H NMR (300 MHz, DMSO, δ (p.p.m.): 9.22 (*s*, 1H, C17H═N); 8.61 (*d*, 1H, C3H, *J* = 6.24 Hz); 8.00 (*d*, 2H, C11H, C15H, *J* = 7.26 Hz); 7.90 (*d*, 1H, C6H, *J* = 4.95); 7.49 (*t*, 8H, C1H, C2H, C12H, C13H, C14H, C20H, C21H, C22H); *m*/*z* (*M*+1): 304. IR (KBr): ν(CH═N, imine) = 1560 cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The reflections (0 1 1) and (0 0 1) affected by the beam-stop were removed during refinement.

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full crystallographic data

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Crystal data

$C_{18}H_{13}N_3S$
M_r = 303.37
Triclinic, $P\overline{1}$
a = 9.6524 (17) Å
b = 10.1168 (17) Å
c = 16.655 (3) Å
α = 101.299 (8)°
β = 106.315 (9)°
γ = 95.628 (8)°
V = 1510.3 (5) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8471 reflections
θ = 2.1–29.6°
μ = 0.21 mm^{-1}
T = 296 K
Parallelepiped, yellow
0.44 × 0.21 × 0.12 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.641, T_{max} = 0.746
66495 measured reflections
8471 independent reflections
5839 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 29.6°, θ_{min} = 2.1°
h = −13→13
k = −14→14
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.02
8471 reflections
397 parameters
0 restraints
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2 + 0.3505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.17058 (19)	1.07411 (19)	0.26058 (13)	0.0566 (5)
H1	0.0964	1.1046	0.2811	0.068*
C2	0.17571 (19)	1.07047 (19)	0.18053 (12)	0.0553 (4)
H2	0.1049	1.0979	0.1392	0.066*
C3	0.29993 (18)	1.02058 (17)	0.16562 (11)	0.0450 (4)
H3	0.3202	1.0120	0.1136	0.054*
C4	0.38753 (16)	0.98610 (14)	0.23621 (9)	0.0358 (3)
C5	0.51463 (16)	0.92090 (15)	0.24091 (10)	0.0394 (3)
H5	0.5508	0.9077	0.1943	0.047*
C6	0.68652 (15)	0.80001 (14)	0.31175 (9)	0.0351 (3)
C7	0.67572 (17)	0.76611 (17)	0.45524 (10)	0.0438 (4)
H7	0.6157	0.8308	0.4630	0.053*
C8	0.72008 (18)	0.69263 (18)	0.51458 (10)	0.0487 (4)
H8	0.6906	0.7071	0.5637	0.058*
C9	0.81108 (18)	0.59378 (17)	0.50265 (10)	0.0465 (4)
H9	0.8398	0.5431	0.5436	0.056*
C10	0.85662 (16)	0.57250 (16)	0.43193 (10)	0.0420 (3)
H10	0.9171	0.5080	0.4245	0.050*
C11	0.81172 (15)	0.64882 (15)	0.36971 (9)	0.0355 (3)
C12	0.76267 (15)	0.73725 (14)	0.25917 (9)	0.0349 (3)
C13	0.76897 (16)	0.75279 (15)	0.17423 (9)	0.0371 (3)
C14	0.78455 (18)	0.87931 (16)	0.15375 (11)	0.0445 (4)
H14	0.7897	0.9584	0.1946	0.053*
C15	0.7924 (2)	0.88867 (19)	0.07363 (12)	0.0545 (4)
H15	0.8021	0.9738	0.0607	0.065*
C16	0.7860 (2)	0.7727 (2)	0.01279 (12)	0.0618 (5)
H16	0.7900	0.7791	−0.0415	0.074*
C17	0.7738 (3)	0.6472 (2)	0.03267 (12)	0.0695 (6)
H17	0.7713	0.5688	−0.0080	0.083*
C18	0.7651 (2)	0.63667 (18)	0.11265 (11)	0.0551 (5)
H18	0.7565	0.5513	0.1254	0.066*
C19	0.15325 (19)	0.58262 (18)	0.24891 (12)	0.0537 (4)
H19	0.0670	0.6036	0.2590	0.064*
C20	0.21283 (19)	0.63493 (17)	0.19618 (11)	0.0504 (4)
H20	0.1724	0.6964	0.1653	0.060*
C21	0.34351 (18)	0.58659 (17)	0.19260 (11)	0.0469 (4)
H21	0.3987	0.6131	0.1591	0.056*
C22	0.38076 (16)	0.49675 (15)	0.24342 (9)	0.0358 (3)
C23	0.50661 (16)	0.42895 (15)	0.25537 (10)	0.0387 (3)
H23	0.5732	0.4454	0.2261	0.046*
C24	0.65015 (15)	0.28079 (14)	0.31498 (9)	0.0354 (3)
C25	0.64809 (18)	0.25257 (17)	0.46057 (10)	0.0463 (4)
H25	0.5669	0.2949	0.4610	0.056*
C26	0.7178 (2)	0.20410 (19)	0.52865 (11)	0.0528 (4)
H26	0.6829	0.2111	0.5758	0.063*

C27	0.8433 (2)	0.14293 (19)	0.52856 (12)	0.0547 (4)
H27	0.8905	0.1103	0.5758	0.066*
C28	0.89535 (18)	0.13129 (17)	0.46045 (11)	0.0492 (4)
H28	0.9784	0.0916	0.4610	0.059*
C29	0.82264 (16)	0.17983 (15)	0.38854 (10)	0.0383 (3)
C30	0.74535 (15)	0.24182 (14)	0.26932 (9)	0.0357 (3)
C31	0.74357 (16)	0.25291 (15)	0.18214 (10)	0.0376 (3)
C32	0.61448 (19)	0.22930 (18)	0.11395 (10)	0.0498 (4)
H32	0.5251	0.2085	0.1233	0.060*
C33	0.6181 (2)	0.2365 (2)	0.03260 (11)	0.0607 (5)
H33	0.5312	0.2206	−0.0124	0.073*
C34	0.7490 (2)	0.26692 (19)	0.01772 (12)	0.0608 (5)
H34	0.7510	0.2719	−0.0371	0.073*
C35	0.8771 (2)	0.28999 (19)	0.08419 (13)	0.0578 (5)
H35	0.9659	0.3111	0.0743	0.069*
C36	0.87527 (18)	0.28216 (17)	0.16590 (11)	0.0480 (4)
H36	0.9629	0.2966	0.2103	0.058*
N1	0.57877 (13)	0.88081 (12)	0.30812 (8)	0.0384 (3)
N2	0.72080 (12)	0.74350 (12)	0.38341 (7)	0.0349 (3)
N3	0.83822 (13)	0.64448 (13)	0.29550 (8)	0.0385 (3)
N4	0.52949 (13)	0.34609 (13)	0.30544 (8)	0.0389 (3)
N5	0.69919 (13)	0.23822 (12)	0.39100 (8)	0.0358 (3)
N6	0.85190 (14)	0.18142 (13)	0.31564 (8)	0.0416 (3)
S1	0.31655 (5)	1.01616 (5)	0.32036 (3)	0.04986 (13)
S2	0.25440 (5)	0.47252 (5)	0.29562 (3)	0.06015 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0449 (9)	0.0673 (11)	0.0729 (12)	0.0299 (8)	0.0284 (9)	0.0261 (10)
C2	0.0416 (9)	0.0683 (11)	0.0637 (11)	0.0266 (8)	0.0135 (8)	0.0288 (9)
C3	0.0461 (9)	0.0519 (9)	0.0440 (9)	0.0186 (7)	0.0162 (7)	0.0188 (7)
C4	0.0365 (7)	0.0354 (7)	0.0411 (8)	0.0135 (6)	0.0150 (6)	0.0133 (6)
C5	0.0414 (8)	0.0436 (8)	0.0402 (8)	0.0186 (6)	0.0178 (6)	0.0129 (6)
C6	0.0353 (7)	0.0388 (7)	0.0350 (7)	0.0145 (6)	0.0121 (6)	0.0112 (6)
C7	0.0441 (8)	0.0555 (9)	0.0407 (8)	0.0222 (7)	0.0208 (7)	0.0136 (7)
C8	0.0492 (9)	0.0662 (11)	0.0403 (8)	0.0203 (8)	0.0202 (7)	0.0196 (8)
C9	0.0443 (9)	0.0593 (10)	0.0441 (9)	0.0180 (7)	0.0143 (7)	0.0254 (8)
C10	0.0375 (8)	0.0491 (9)	0.0450 (8)	0.0186 (7)	0.0121 (6)	0.0188 (7)
C11	0.0313 (7)	0.0406 (7)	0.0388 (8)	0.0144 (6)	0.0122 (6)	0.0123 (6)
C12	0.0336 (7)	0.0381 (7)	0.0362 (7)	0.0138 (6)	0.0118 (6)	0.0108 (6)
C13	0.0361 (7)	0.0433 (8)	0.0376 (7)	0.0155 (6)	0.0149 (6)	0.0128 (6)
C14	0.0475 (9)	0.0436 (8)	0.0486 (9)	0.0132 (7)	0.0208 (7)	0.0138 (7)
C15	0.0583 (11)	0.0594 (11)	0.0618 (11)	0.0183 (9)	0.0289 (9)	0.0321 (9)
C16	0.0769 (13)	0.0819 (13)	0.0482 (10)	0.0350 (11)	0.0344 (10)	0.0316 (10)
C17	0.1087 (18)	0.0660 (12)	0.0474 (10)	0.0396 (12)	0.0364 (11)	0.0143 (9)
C18	0.0849 (13)	0.0458 (9)	0.0465 (9)	0.0279 (9)	0.0294 (9)	0.0158 (8)
C19	0.0444 (9)	0.0609 (11)	0.0660 (11)	0.0270 (8)	0.0232 (8)	0.0203 (9)

C20	0.0507 (9)	0.0506 (9)	0.0556 (10)	0.0228 (8)	0.0141 (8)	0.0218 (8)
C21	0.0479 (9)	0.0520 (9)	0.0519 (9)	0.0164 (7)	0.0218 (8)	0.0245 (8)
C22	0.0350 (7)	0.0393 (7)	0.0351 (7)	0.0098 (6)	0.0124 (6)	0.0092 (6)
C23	0.0345 (7)	0.0420 (8)	0.0433 (8)	0.0105 (6)	0.0146 (6)	0.0128 (6)
C24	0.0324 (7)	0.0387 (7)	0.0371 (7)	0.0094 (6)	0.0101 (6)	0.0127 (6)
C25	0.0472 (9)	0.0529 (9)	0.0465 (9)	0.0130 (7)	0.0214 (7)	0.0169 (7)
C26	0.0610 (11)	0.0608 (10)	0.0435 (9)	0.0105 (9)	0.0206 (8)	0.0207 (8)
C27	0.0575 (10)	0.0612 (11)	0.0479 (10)	0.0102 (9)	0.0092 (8)	0.0281 (8)
C28	0.0435 (9)	0.0555 (10)	0.0531 (10)	0.0161 (7)	0.0108 (7)	0.0253 (8)
C29	0.0348 (7)	0.0384 (7)	0.0427 (8)	0.0098 (6)	0.0098 (6)	0.0130 (6)
C30	0.0327 (7)	0.0377 (7)	0.0385 (8)	0.0103 (6)	0.0108 (6)	0.0110 (6)
C31	0.0409 (8)	0.0375 (7)	0.0405 (8)	0.0146 (6)	0.0169 (6)	0.0129 (6)
C32	0.0461 (9)	0.0614 (10)	0.0421 (9)	0.0090 (8)	0.0145 (7)	0.0111 (8)
C33	0.0685 (12)	0.0732 (12)	0.0387 (9)	0.0171 (10)	0.0125 (9)	0.0122 (9)
C34	0.0918 (15)	0.0595 (11)	0.0489 (10)	0.0305 (10)	0.0372 (10)	0.0221 (9)
C35	0.0667 (12)	0.0613 (11)	0.0709 (12)	0.0275 (9)	0.0448 (10)	0.0313 (10)
C36	0.0446 (9)	0.0527 (9)	0.0574 (10)	0.0192 (7)	0.0227 (8)	0.0216 (8)
N1	0.0373 (6)	0.0397 (6)	0.0426 (7)	0.0183 (5)	0.0138 (5)	0.0115 (5)
N2	0.0332 (6)	0.0419 (7)	0.0348 (6)	0.0165 (5)	0.0126 (5)	0.0124 (5)
N3	0.0373 (6)	0.0457 (7)	0.0398 (7)	0.0200 (5)	0.0151 (5)	0.0154 (5)
N4	0.0350 (6)	0.0454 (7)	0.0402 (7)	0.0148 (5)	0.0131 (5)	0.0126 (6)
N5	0.0347 (6)	0.0387 (6)	0.0366 (6)	0.0093 (5)	0.0116 (5)	0.0123 (5)
N6	0.0389 (7)	0.0471 (7)	0.0440 (7)	0.0171 (6)	0.0138 (6)	0.0162 (6)
S1	0.0535 (3)	0.0629 (3)	0.0473 (2)	0.0285 (2)	0.02553 (19)	0.0213 (2)
S2	0.0585 (3)	0.0798 (3)	0.0735 (3)	0.0368 (2)	0.0419 (2)	0.0458 (3)

Geometric parameters (Å, º)

C1—C2	1.341 (3)	C19—C20	1.337 (2)
C1—S1	1.7096 (17)	C19—S2	1.7105 (17)
C1—H1	0.9300	C19—H19	0.9300
C2—C3	1.411 (2)	C20—C21	1.409 (2)
C2—H2	0.9300	C20—H20	0.9300
C3—C4	1.371 (2)	C21—C22	1.366 (2)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.4392 (19)	C22—C23	1.4376 (19)
C4—S1	1.7145 (15)	C22—S2	1.7100 (15)
C5—N1	1.2801 (18)	C23—N4	1.2860 (18)
C5—H5	0.9300	C23—H23	0.9300
C6—N1	1.3799 (17)	C24—N4	1.3806 (18)
C6—N2	1.3941 (18)	C24—C30	1.387 (2)
C6—C12	1.395 (2)	C24—N5	1.3891 (18)
C7—C8	1.351 (2)	C25—C26	1.354 (2)
C7—N2	1.3703 (19)	C25—N5	1.3697 (19)
C7—H7	0.9300	C25—H25	0.9300
C8—C9	1.415 (2)	C26—C27	1.413 (3)
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.355 (2)	C27—C28	1.354 (2)

C9—H9	0.9300	C27—H27	0.9300
C10—C11	1.4088 (19)	C28—C29	1.412 (2)
C10—H10	0.9300	C28—H28	0.9300
C11—N3	1.3242 (18)	C29—N6	1.324 (2)
C11—N2	1.3898 (17)	C29—N5	1.3880 (18)
C12—N3	1.3739 (17)	C30—N6	1.3743 (18)
C12—C13	1.471 (2)	C30—C31	1.473 (2)
C13—C18	1.390 (2)	C31—C36	1.388 (2)
C13—C14	1.393 (2)	C31—C32	1.393 (2)
C14—C15	1.379 (2)	C32—C33	1.381 (2)
C14—H14	0.9300	C32—H32	0.9300
C15—C16	1.376 (3)	C33—C34	1.372 (3)
C15—H15	0.9300	C33—H33	0.9300
C16—C17	1.376 (3)	C34—C35	1.372 (3)
C16—H16	0.9300	C34—H34	0.9300
C17—C18	1.382 (2)	C35—C36	1.383 (2)
C17—H17	0.9300	C35—H35	0.9300
C18—H18	0.9300	C36—H36	0.9300

C2—C1—S1	112.04 (13)	C22—C21—C20	113.05 (15)
C2—C1—H1	124.0	C22—C21—H21	123.5
S1—C1—H1	124.0	C20—C21—H21	123.5
C1—C2—C3	112.84 (15)	C21—C22—C23	127.71 (14)
C1—C2—H2	123.6	C21—C22—S2	110.50 (11)
C3—C2—H2	123.6	C23—C22—S2	121.79 (11)
C4—C3—C2	112.60 (15)	N4—C23—C22	121.71 (14)
C4—C3—H3	123.7	N4—C23—H23	119.1
C2—C3—H3	123.7	C22—C23—H23	119.1
C3—C4—C5	127.09 (14)	N4—C24—C30	138.57 (13)
C3—C4—S1	110.75 (11)	N4—C24—N5	116.60 (13)
C5—C4—S1	121.90 (11)	C30—C24—N5	104.83 (12)
N1—C5—C4	121.22 (14)	C26—C25—N5	118.84 (16)
N1—C5—H5	119.4	C26—C25—H25	120.6
C4—C5—H5	119.4	N5—C25—H25	120.6
N1—C6—N2	114.96 (12)	C25—C26—C27	120.38 (17)
N1—C6—C12	139.56 (13)	C25—C26—H26	119.8
N2—C6—C12	104.65 (11)	C27—C26—H26	119.8
C8—C7—N2	118.79 (14)	C28—C27—C26	120.69 (15)
C8—C7—H7	120.6	C28—C27—H27	119.7
N2—C7—H7	120.6	C26—C27—H27	119.7
C7—C8—C9	120.61 (15)	C27—C28—C29	119.54 (16)
C7—C8—H8	119.7	C27—C28—H28	120.2
C9—C8—H8	119.7	C29—C28—H28	120.2
C10—C9—C8	120.48 (14)	N6—C29—N5	111.06 (12)
C10—C9—H9	119.8	N6—C29—C28	131.03 (15)
C8—C9—H9	119.8	N5—C29—C28	117.90 (14)
C9—C10—C11	119.51 (14)	N6—C30—C24	110.99 (13)
C9—C10—H10	120.2	N6—C30—C31	119.15 (12)

C11—C10—H10	120.2	C24—C30—C31	129.83 (13)
N3—C11—N2	111.13 (12)	C36—C31—C32	118.32 (15)
N3—C11—C10	130.72 (13)	C36—C31—C30	119.20 (14)
N2—C11—C10	118.12 (13)	C32—C31—C30	122.42 (14)
N3—C12—C6	110.91 (13)	C33—C32—C31	120.55 (17)
N3—C12—C13	118.49 (12)	C33—C32—H32	119.7
C6—C12—C13	130.57 (12)	C31—C32—H32	119.7
C18—C13—C14	118.35 (14)	C34—C33—C32	120.47 (18)
C18—C13—C12	118.66 (14)	C34—C33—H33	119.8
C14—C13—C12	122.94 (14)	C32—C33—H33	119.8
C15—C14—C13	120.75 (16)	C35—C34—C33	119.64 (17)
C15—C14—H14	119.6	C35—C34—H34	120.2
C13—C14—H14	119.6	C33—C34—H34	120.2
C16—C15—C14	120.28 (16)	C34—C35—C36	120.55 (17)
C16—C15—H15	119.9	C34—C35—H35	119.7
C14—C15—H15	119.9	C36—C35—H35	119.7
C15—C16—C17	119.66 (17)	C35—C36—C31	120.47 (16)
C15—C16—H16	120.2	C35—C36—H36	119.8
C17—C16—H16	120.2	C31—C36—H36	119.8
C16—C17—C18	120.48 (18)	C5—N1—C6	123.72 (13)
C16—C17—H17	119.8	C7—N2—C11	122.48 (12)
C18—C17—H17	119.8	C7—N2—C6	130.34 (12)
C17—C18—C13	120.45 (16)	C11—N2—C6	107.15 (11)
C17—C18—H18	119.8	C11—N3—C12	106.14 (12)
C13—C18—H18	119.8	C23—N4—C24	120.64 (13)
C20—C19—S2	111.98 (13)	C25—N5—C29	122.62 (13)
C20—C19—H19	124.0	C25—N5—C24	130.14 (13)
S2—C19—H19	124.0	C29—N5—C24	107.17 (12)
C19—C20—C21	112.60 (15)	C29—N6—C30	105.92 (12)
C19—C20—H20	123.7	C1—S1—C4	91.78 (8)
C21—C20—H20	123.7	C22—S2—C19	91.88 (8)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C31–C36 and C13–C18 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···N3^{i}	0.93	2.50	3.428 (2)	175
C14—H14···N6^{ii}	0.93	2.61	3.526 (2)	170
C15—H15···*Cg*1^{ii}	0.93	2.97	3.778 (2)	146
C18—H18···*Cg*1	0.93	2.88	3.761 (2)	157
C33—H33···*Cg*2^{iii}	0.93	2.95	3.814 (2)	155

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