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(E)-2-Benzoyl-3-[1-phenyl-3-(thiophen-2-yl)-1H-pyrazol-4-yl]acrylonitrile

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The asymmetric unit of the title compound, $C_{23}H_{15}N_3OS$, consists of two crystallographically independent molecules, which are related by a pseudo-inversion centre. In one molecule, the pyrazolyl ring makes dihedral angles of 35.7 (4), 19.1 (1) and 47.3 (1)°, respectively, with the thiophenyl ring, the attached phenyl ring and the phenyl ring of the benzoyl group. In the second molecule, the corresponding values are 37.4 (1), 16.1 (1) and 48.2 (1)°, respectively. In the crystal, the two independent molecules are linked to each other via a π–π interaction between the pyrazolyl rings [centroid–centroid distance = 3.578 (12) Å]. Weak intermolecular C—H···O interactions are also observed. The thiophenyl ring of one molecule is disordered over two orientations, with a refined occupancy ratio of 0.768 (3):0.232 (3).

3D view
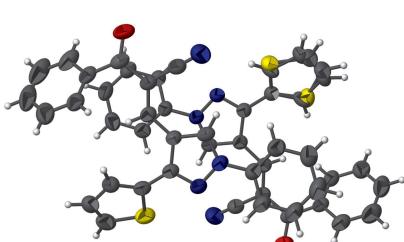
Chemical scheme
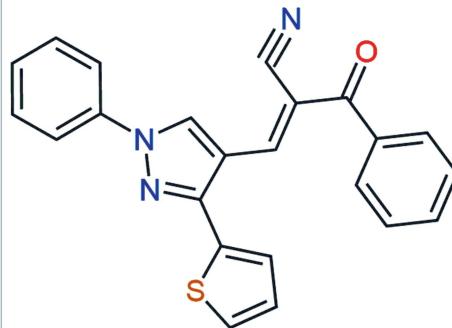
Structure description

3-(2′-Thienyl)pyrazole-based heterocycles show various biological applications with antimicrobial, antioxidant, anti-inflammatory and analgesic activities (Abdel-Wahab et al., 2011, 2012; Naim et al., 2016). Various synthetic approaches have been reported for the formation of heterocycles containing thiophene and pyrazole moieties (Abdel-Wahab et al., 2010; Bratenko et al., 2005).

The asymmetric unit consists of two unique molecules, which are related to each other by a pseudo-inversion centre (Fig. 1). The N1/N2/C7–C9 pyrazolyl ring makes dihedral angles of 35.7 (4), 19.1 (1) and 47.3 (1)°, respectively, with the S1/C10–C13 thiophenyl
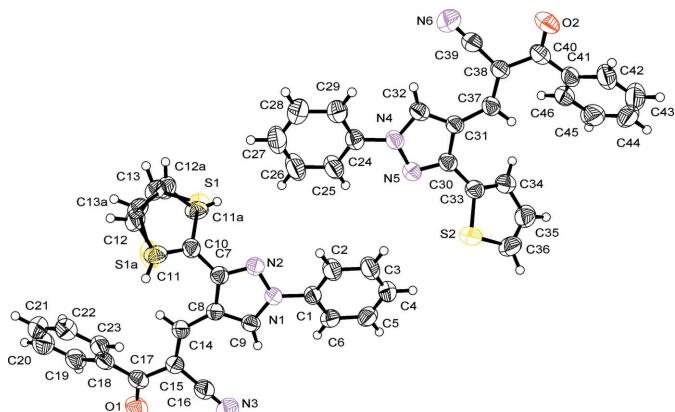
Figure 1
The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

ring, the C1–C6 and C18–C23 phenyl rings, while the N4/N5/C30–C32 pyrazolyl ring makes dihedral angles of 37.4 (1), 16.1 (1) and 48.2 (1)°, respectively, with the S2/C33–C36, C24–C29 and C41–C46 rings.

In the crystal, the two independent molecules are linked through a π–π interaction between the pyrazolyl rings with a centroid–centroid distance of 3.578 (12) Å (Fig. 2). Weak intermolecular C—H···O hydrogen bonds (Table 1) are also observed.

Synthesis and crystallization

The title compound was synthesized from reaction of a mixture of 1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbaldehyde and 3-oxo-3-phenylpropanenitrile in dry ethanol containing piperidine as a catalyst. The solution was refluxed for 5 h. The solid obtained was filtrated and dried. Yellow in CIF single crystals suitable for X-ray diffraction were obtained
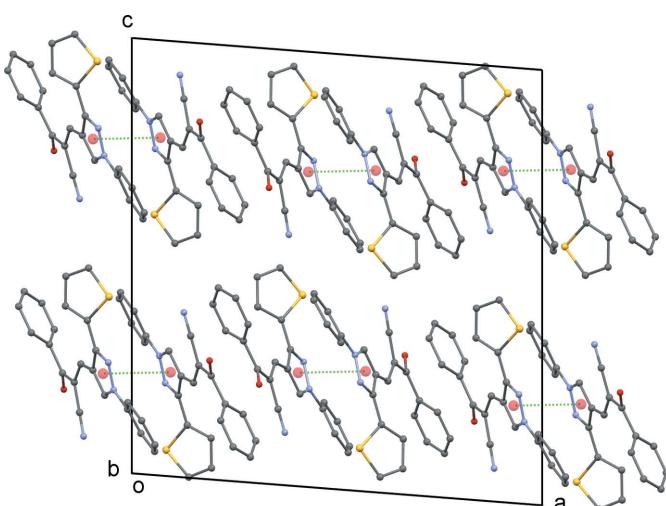

Figure 2
A packing diagram viewed along the b axis. π–π interactions are shown as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C34—H34···O2^i	0.93	2.61	3.396 (3)	143
C46—H46···O2^i	0.93	2.45	3.363 (3)	167

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{15}N_3OS$
M_r	381.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	19.2666 (10), 9.7769 (4), 20.3265 (12)
β (°)	94.423 (5)
V (Å^3)	3817.5 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.28 × 0.15 × 0.06
Data collection	
Diffractometer	Rigaku Oxford Diffraction Super-Nova, Dual, Cu at zero, Atlas
Absorption correction	Numerical (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.563, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22054, 9267, 4750
R_{int}	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.167, 1.02
No. of reflections	9267
No. of parameters	524
No. of restraints	30
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.30

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

from an ethanol solution [yield 79%, m.p. 182–184°C; reported m.p. 182–184°C (Abdel-Wahab *et al.*, 2017)].

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The thiophenyl ring (S1/C10–C13) of one molecule is disordered over two orientations around the C7—C10 bond. The occupancies refined to 0.768 (3) and 0.232 (3). Both major and minor components were restrained to have similar geometries and the anisotropic displacement parameters of C atoms of the minor component were constrained to be the same as those of the major component.

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full crystallographic data

(*E*)-2-Benzoyl-3-[1-phenyl-3-(thiophen-2-yl)-1*H*-pyrazol-4-yl]acrylonitrile

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(*E*)-2-Benzoyl-3-[1-phenyl-3-(thiophen-2-yl)-1*H*-pyrazol-4-yl]acrylonitrile

Crystal data

$C_{23}H_{15}N_3OS$	$F(000) = 1584$
$M_r = 381.44$	$D_x = 1.327$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 19.2666$ (10) Å	Cell parameters from 4056 reflections
$b = 9.7769$ (4) Å	$\theta = 3.5$–26.2°
$c = 20.3265$ (12) Å	$\mu = 0.19$ mm^{-1}
$\beta = 94.423$ (5)°	$T = 296$ K
$V = 3817.5$ (3) Å^3	Plate, yellow
$Z = 8$	$0.28 \times 0.15 \times 0.06$ mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer	22054 measured reflections
	9267 independent reflections
	4750 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.038$
Absorption correction: numerical (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)	$\theta_{max} = 29.9°$, $\theta_{min} = 2.9°$
	$h = -19 \rightarrow 26$
	$k = -12 \rightarrow 13$
$T_{min} = 0.563$, $T_{max} = 0.990$	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.167$	$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.3861P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
9267 reflections	$(\Delta/\sigma)_{max} < 0.001$
524 parameters	$\Delta\rho_{max} = 0.16$ e Å^{-3}
30 restraints	$\Delta\rho_{min} = -0.30$ 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	$U_{iso}*/U_{eq}$	Occ. (<1)
C1	−0.01004 (11)	−0.0978 (2)	0.14670 (12)	0.0454 (5)	
C2	−0.00943 (13)	−0.2356 (2)	0.16190 (14)	0.0609 (7)	
H2	−0.031422	−0.267522	0.198053	0.073*	
C3	0.02426 (14)	−0.3250 (3)	0.12271 (15)	0.0695 (8)	
H3	0.024800	−0.417852	0.132607	0.083*	
C4	0.05675 (14)	−0.2795 (3)	0.06974 (14)	0.0650 (7)	
H4	0.079374	−0.340837	0.043723	0.078*	
C5	0.05588 (13)	−0.1424 (3)	0.05496 (13)	0.0626 (7)	
H5	0.077931	−0.111057	0.018732	0.075*	
C6	0.02243 (12)	−0.0504 (2)	0.09361 (12)	0.0551 (6)	
H6	0.022041	0.042453	0.083616	0.066*	
C7	−0.08758 (11)	0.0626 (2)	0.27623 (12)	0.0449 (5)	
C8	−0.09450 (11)	0.1731 (2)	0.23004 (11)	0.0441 (5)	
C9	−0.06568 (11)	0.1226 (2)	0.17469 (12)	0.0465 (5)	
H9	−0.061972	0.169013	0.135190	0.056*	
C10	−0.10581 (12)	0.0561 (2)	0.34403 (12)	0.0481 (6)	0.768 (3)
C11	−0.1596 (6)	0.1225 (13)	0.3717 (5)	0.062 (3)	0.768 (3)
H11	−0.191951	0.178354	0.348419	0.075*	0.768 (3)
C12	−0.1591 (3)	0.0939 (6)	0.4414 (3)	0.0722 (15)	0.768 (3)
H12	−0.192933	0.124859	0.468043	0.087*	0.768 (3)
C13	−0.1036 (3)	0.0167 (6)	0.4635 (2)	0.0678 (14)	0.768 (3)
H13	−0.093513	−0.007245	0.507529	0.081*	0.768 (3)
S1	−0.05506 (10)	−0.03086 (17)	0.40164 (7)	0.0597 (4)	0.768 (3)
C10A	−0.10581 (12)	0.0561 (2)	0.34403 (12)	0.0481 (6)	0.232 (3)
C11A	−0.0610 (12)	−0.009 (3)	0.3929 (9)	0.062 (3)	0.232 (3)
H11A	−0.018667	−0.049121	0.384726	0.075*	0.232 (3)
C12A	−0.0885 (13)	−0.007 (3)	0.4559 (9)	0.0722 (15)	0.232 (3)
H12A	−0.068910	−0.051770	0.493105	0.087*	0.232 (3)
C13A	−0.1462 (13)	0.070 (3)	0.4546 (9)	0.0678 (14)	0.232 (3)
H13A	−0.169438	0.091173	0.491652	0.081*	0.232 (3)
S1A	−0.1719 (7)	0.1219 (13)	0.3767 (6)	0.078 (3)	0.232 (3)
C14	−0.12398 (11)	0.3051 (2)	0.24226 (12)	0.0470 (5)	
H14	−0.133136	0.322213	0.285753	0.056*	
C15	−0.14026 (11)	0.4081 (2)	0.19891 (12)	0.0481 (6)	
C16	−0.12709 (14)	0.3971 (2)	0.13089 (16)	0.0611 (7)	
C17	−0.16859 (12)	0.5420 (2)	0.21806 (13)	0.0516 (6)	
C18	−0.20071 (12)	0.5570 (2)	0.28148 (12)	0.0513 (6)	
C19	−0.18888 (14)	0.6776 (2)	0.31687 (14)	0.0632 (7)	
H19	−0.160196	0.744603	0.301042	0.076*	
C20	−0.21904 (16)	0.6985 (3)	0.37465 (16)	0.0778 (9)	
H20	−0.210875	0.779466	0.397992	0.093*	
C21	−0.26172 (16)	0.5994 (3)	0.39848 (15)	0.0788 (9)	
H21	−0.281367	0.612784	0.438361	0.095*	
C22	−0.27520 (14)	0.4806 (3)	0.36313 (15)	0.0681 (7)	
H22	−0.304895	0.415018	0.378622	0.082*	

C23	−0.24482 (12)	0.4590 (2)	0.30512 (13)	0.0550 (6)
H23	−0.253778	0.378644	0.281531	0.066*
C24	0.03423 (11)	0.3885 (2)	0.31778 (13)	0.0498 (6)
C25	0.03157 (13)	0.5267 (2)	0.30351 (15)	0.0671 (8)
H25	0.051478	0.560383	0.266545	0.081*
C26	−0.00072 (16)	0.6135 (3)	0.34441 (18)	0.0842 (9)
H26	−0.002661	0.706520	0.334874	0.101*
C27	−0.03021 (15)	0.5654 (3)	0.39917 (17)	0.0810 (9)
H27	−0.052164	0.625314	0.426430	0.097*
C28	−0.02707 (14)	0.4271 (3)	0.41355 (15)	0.0735 (8)
H28	−0.046752	0.393605	0.450686	0.088*
C29	0.00541 (13)	0.3389 (3)	0.37257 (14)	0.0624 (7)
H29	0.007715	0.245937	0.382144	0.075*
C30	0.11350 (11)	0.2360 (2)	0.18758 (12)	0.0464 (6)
C31	0.12010 (11)	0.1233 (2)	0.23240 (11)	0.0436 (5)
C32	0.09022 (11)	0.1702 (2)	0.28749 (12)	0.0487 (6)
H32	0.086479	0.121975	0.326511	0.058*
C33	0.13532 (12)	0.2442 (2)	0.12074 (12)	0.0505 (6)
C34	0.19299 (13)	0.1889 (2)	0.09487 (13)	0.0572 (6)
H34	0.227400	0.140826	0.119763	0.069*
C35	0.19433 (15)	0.2129 (3)	0.02682 (14)	0.0685 (7)
H35	0.229768	0.182593	0.001853	0.082*
C36	0.13861 (17)	0.2847 (3)	0.00160 (14)	0.0760 (8)
H36	0.131071	0.308578	−0.042657	0.091*
C37	0.15047 (11)	−0.0068 (2)	0.21921 (12)	0.0468 (6)
H37	0.163354	−0.018387	0.176400	0.056*
C38	0.16320 (11)	−0.1154 (2)	0.25979 (12)	0.0473 (6)
C39	0.14342 (13)	−0.1151 (2)	0.32593 (15)	0.0560 (6)
C40	0.19362 (12)	−0.2461 (2)	0.23808 (13)	0.0528 (6)
C41	0.22781 (12)	−0.2530 (2)	0.17564 (13)	0.0537 (6)
C42	0.21698 (15)	−0.3699 (3)	0.13695 (17)	0.0753 (9)
H42	0.189011	−0.440018	0.150910	0.090*
C43	0.2470 (2)	−0.3818 (4)	0.0791 (2)	0.1062 (13)
H43	0.239296	−0.459619	0.053271	0.127*
C44	0.2886 (2)	−0.2794 (5)	0.05866 (17)	0.1052 (13)
H44	0.308100	−0.287526	0.018394	0.126*
C45	0.30226 (16)	−0.1632 (4)	0.09698 (17)	0.0849 (9)
H45	0.331730	−0.095273	0.083306	0.102*
C46	0.27149 (13)	−0.1507 (3)	0.15529 (14)	0.0600 (7)
H46	0.279869	−0.073400	0.181363	0.072*
N1	−0.04409 (9)	−0.00525 (17)	0.18823 (9)	0.0455 (5)
N2	−0.05719 (9)	−0.04497 (17)	0.25023 (10)	0.0480 (5)
N3	−0.11748 (15)	0.3875 (2)	0.07645 (14)	0.0903 (8)
N4	0.06743 (9)	0.29801 (17)	0.27477 (10)	0.0487 (5)
N5	0.08151 (10)	0.34125 (18)	0.21337 (10)	0.0502 (5)
N6	0.12700 (14)	−0.1138 (2)	0.37868 (14)	0.0815 (7)
O1	−0.16545 (9)	0.63946 (16)	0.18061 (10)	0.0706 (5)
O2	0.18950 (10)	−0.34754 (16)	0.27296 (10)	0.0746 (6)

| S2 | 0.08406 (4) | 0.32604 (7) | 0.05995 (4) | 0.0704 (2) |

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0443 (12)	0.0460 (12)	0.0456 (15)	0.0044 (10)	0.0016 (11)	−0.0034 (11)
C2	0.0680 (15)	0.0494 (13)	0.0676 (19)	0.0063 (12)	0.0199 (14)	0.0019 (12)
C3	0.0821 (18)	0.0518 (14)	0.077 (2)	0.0158 (13)	0.0192 (16)	0.0000 (14)
C4	0.0691 (16)	0.0690 (17)	0.0569 (19)	0.0221 (14)	0.0055 (14)	−0.0082 (14)
C5	0.0638 (15)	0.0795 (18)	0.0451 (16)	0.0082 (14)	0.0082 (13)	0.0000 (13)
C6	0.0657 (15)	0.0531 (13)	0.0462 (16)	0.0023 (12)	0.0019 (13)	0.0037 (12)
C7	0.0460 (12)	0.0427 (11)	0.0458 (15)	−0.0004 (10)	0.0031 (11)	0.0003 (10)
C8	0.0477 (12)	0.0421 (11)	0.0420 (14)	0.0023 (10)	0.0000 (10)	0.0001 (10)
C9	0.0512 (13)	0.0416 (11)	0.0460 (15)	0.0024 (10)	0.0001 (11)	0.0051 (10)
C10	0.0546 (13)	0.0415 (11)	0.0489 (16)	0.0006 (10)	0.0092 (12)	0.0000 (10)
C11	0.059 (5)	0.075 (5)	0.054 (4)	0.005 (3)	0.015 (3)	0.025 (3)
C12	0.094 (4)	0.068 (3)	0.060 (4)	0.010 (2)	0.039 (3)	0.011 (2)
C13	0.093 (5)	0.068 (4)	0.044 (2)	0.006 (3)	0.014 (2)	0.002 (2)
S1	0.0714 (7)	0.0573 (7)	0.0508 (8)	0.0087 (5)	0.0071 (6)	0.0099 (5)
C10A	0.0546 (13)	0.0415 (11)	0.0489 (16)	0.0006 (10)	0.0092 (12)	0.0000 (10)
C11A	0.059 (5)	0.075 (5)	0.054 (4)	0.005 (3)	0.015 (3)	0.025 (3)
C12A	0.094 (4)	0.068 (3)	0.060 (4)	0.010 (2)	0.039 (3)	0.011 (2)
C13A	0.093 (5)	0.068 (4)	0.044 (2)	0.006 (3)	0.014 (2)	0.002 (2)
S1A	0.071 (4)	0.069 (4)	0.098 (6)	0.006 (3)	0.036 (3)	−0.001 (3)
C14	0.0519 (13)	0.0425 (11)	0.0463 (15)	0.0017 (10)	0.0010 (11)	−0.0027 (10)
C15	0.0533 (13)	0.0440 (12)	0.0468 (16)	0.0025 (10)	0.0033 (11)	0.0020 (11)
C16	0.0728 (17)	0.0510 (14)	0.060 (2)	0.0088 (12)	0.0102 (15)	0.0090 (13)
C17	0.0521 (13)	0.0418 (12)	0.0597 (17)	0.0001 (10)	−0.0035 (12)	0.0029 (12)
C18	0.0559 (14)	0.0411 (11)	0.0558 (17)	0.0089 (11)	−0.0029 (12)	0.0015 (11)
C19	0.0741 (17)	0.0475 (13)	0.067 (2)	0.0061 (12)	−0.0048 (15)	−0.0047 (13)
C20	0.097 (2)	0.0625 (17)	0.072 (2)	0.0120 (16)	−0.0090 (18)	−0.0148 (16)
C21	0.090 (2)	0.091 (2)	0.0546 (19)	0.0268 (18)	0.0018 (16)	−0.0118 (17)
C22	0.0669 (16)	0.0693 (17)	0.068 (2)	0.0111 (13)	0.0055 (15)	0.0039 (15)
C23	0.0561 (14)	0.0511 (13)	0.0575 (17)	0.0069 (11)	0.0026 (13)	−0.0037 (12)
C24	0.0474 (12)	0.0457 (12)	0.0557 (17)	0.0015 (10)	0.0007 (12)	−0.0056 (11)
C25	0.0745 (17)	0.0466 (13)	0.082 (2)	0.0090 (13)	0.0182 (16)	0.0003 (13)
C26	0.097 (2)	0.0545 (15)	0.104 (3)	0.0179 (15)	0.027 (2)	−0.0068 (17)
C27	0.084 (2)	0.0729 (19)	0.087 (3)	0.0185 (16)	0.0137 (18)	−0.0224 (17)
C28	0.0761 (18)	0.0809 (19)	0.065 (2)	0.0025 (15)	0.0133 (15)	−0.0117 (16)
C29	0.0709 (16)	0.0534 (14)	0.0627 (19)	−0.0001 (13)	0.0049 (14)	−0.0053 (13)
C30	0.0499 (12)	0.0371 (11)	0.0513 (16)	−0.0006 (10)	−0.0016 (11)	−0.0002 (10)
C31	0.0474 (12)	0.0379 (11)	0.0448 (14)	0.0013 (9)	−0.0009 (11)	−0.0001 (10)
C32	0.0521 (13)	0.0387 (11)	0.0540 (16)	0.0008 (10)	−0.0043 (11)	0.0026 (11)
C33	0.0613 (14)	0.0384 (11)	0.0509 (16)	−0.0025 (11)	−0.0009 (12)	0.0018 (10)
C34	0.0618 (15)	0.0544 (13)	0.0555 (18)	0.0046 (12)	0.0055 (13)	0.0064 (12)
C35	0.0865 (19)	0.0605 (15)	0.061 (2)	−0.0020 (15)	0.0208 (16)	0.0022 (14)
C36	0.116 (2)	0.0663 (17)	0.0457 (18)	−0.0002 (17)	0.0051 (17)	0.0080 (14)
C37	0.0492 (12)	0.0418 (11)	0.0486 (15)	0.0017 (10)	−0.0023 (11)	−0.0041 (10)

C38	0.0507 (13)	0.0399 (11)	0.0504 (16)	0.0028 (10)	−0.0028 (11)	0.0011 (10)
C39	0.0671 (16)	0.0449 (13)	0.0552 (19)	0.0044 (11)	0.0003 (14)	0.0042 (12)
C40	0.0518 (13)	0.0398 (12)	0.0646 (18)	0.0030 (10)	−0.0097 (13)	−0.0004 (12)
C41	0.0552 (14)	0.0476 (13)	0.0558 (17)	0.0141 (11)	−0.0117 (13)	−0.0083 (12)
C42	0.0811 (19)	0.0574 (15)	0.083 (2)	0.0195 (14)	−0.0205 (17)	−0.0231 (15)
C43	0.129 (3)	0.101 (3)	0.083 (3)	0.049 (2)	−0.027 (2)	−0.039 (2)
C44	0.130 (3)	0.135 (3)	0.050 (2)	0.075 (3)	−0.001 (2)	−0.010 (2)
C45	0.083 (2)	0.102 (2)	0.071 (2)	0.0371 (18)	0.0130 (18)	0.0130 (19)
C46	0.0611 (15)	0.0585 (15)	0.0593 (19)	0.0169 (12)	−0.0030 (14)	−0.0008 (13)
N1	0.0512 (10)	0.0408 (9)	0.0447 (13)	0.0035 (8)	0.0040 (9)	0.0014 (9)
N2	0.0565 (11)	0.0417 (10)	0.0464 (13)	0.0013 (9)	0.0077 (9)	0.0032 (9)
N3	0.133 (2)	0.0801 (17)	0.0608 (19)	0.0188 (15)	0.0272 (17)	0.0141 (14)
N4	0.0529 (11)	0.0400 (9)	0.0526 (14)	0.0031 (8)	0.0002 (10)	−0.0029 (9)
N5	0.0584 (11)	0.0415 (10)	0.0504 (14)	0.0036 (9)	0.0023 (10)	0.0014 (9)
N6	0.107 (2)	0.0762 (16)	0.0622 (18)	0.0028 (14)	0.0157 (15)	0.0054 (13)
O1	0.0846 (12)	0.0475 (9)	0.0808 (15)	0.0079 (9)	0.0140 (10)	0.0159 (9)
O2	0.0883 (13)	0.0453 (9)	0.0901 (16)	0.0088 (9)	0.0058 (11)	0.0160 (10)
S2	0.0886 (5)	0.0588 (4)	0.0618 (5)	0.0138 (3)	−0.0064 (4)	0.0098 (3)

Geometric parameters (Å, º)

C1—C6	1.370 (3)	C22—C23	1.372 (4)
C1—C2	1.382 (3)	C22—H22	0.9300
C1—N1	1.431 (3)	C23—H23	0.9300
C2—C3	1.378 (3)	C24—C29	1.371 (3)
C2—H2	0.9300	C24—C25	1.381 (3)
C3—C4	1.361 (4)	C24—N4	1.429 (3)
C3—H3	0.9300	C25—C26	1.371 (4)
C4—C5	1.374 (3)	C25—H25	0.9300
C4—H4	0.9300	C26—C27	1.371 (4)
C5—C6	1.385 (3)	C26—H26	0.9300
C5—H5	0.9300	C27—C28	1.384 (4)
C6—H6	0.9300	C27—H27	0.9300
C7—N2	1.333 (3)	C28—C29	1.382 (4)
C7—C8	1.430 (3)	C28—H28	0.9300
C7—C10	1.450 (3)	C29—H29	0.9300
C7—C10A	1.450 (3)	C30—N5	1.328 (3)
C8—C9	1.384 (3)	C30—C31	1.430 (3)
C8—C14	1.439 (3)	C30—C33	1.455 (3)
C9—N1	1.339 (3)	C31—C32	1.377 (3)
C9—H9	0.9300	C31—C37	1.434 (3)
C10—C11	1.378 (10)	C32—N4	1.343 (3)
C10—S1	1.695 (3)	C32—H32	0.9300
C11—C12	1.444 (10)	C33—C34	1.376 (3)
C11—H11	0.9300	C33—S2	1.719 (2)
C12—C13	1.357 (5)	C34—C35	1.405 (3)
C12—H12	0.9300	C34—H34	0.9300
C13—S1	1.690 (4)	C35—C36	1.350 (4)

C13—H13	0.9300	C35—H35	0.9300
C10A—C11A	1.417 (15)	C36—S2	1.693 (3)
C10A—S1A	1.615 (10)	C36—H36	0.9300
C11A—C12A	1.425 (16)	C37—C38	1.355 (3)
C11A—H11A	0.9300	C37—H37	0.9300
C12A—C13A	1.336 (14)	C38—C39	1.425 (4)
C12A—H12A	0.9300	C38—C40	1.487 (3)
C13A—S1A	1.700 (14)	C39—N6	1.141 (3)
C13A—H13A	0.9300	C40—O2	1.225 (3)
C14—C15	1.359 (3)	C40—C41	1.476 (4)
C14—H14	0.9300	C41—C46	1.391 (3)
C15—C16	1.429 (4)	C41—C42	1.393 (3)
C15—C17	1.482 (3)	C42—C43	1.355 (5)
C16—N3	1.140 (3)	C42—H42	0.9300
C17—O1	1.224 (3)	C43—C44	1.367 (5)
C17—C18	1.480 (3)	C43—H43	0.9300
C18—C23	1.390 (3)	C44—C45	1.391 (5)
C18—C19	1.392 (3)	C44—H44	0.9300
C19—C20	1.365 (4)	C45—C46	1.371 (4)
C19—H19	0.9300	C45—H45	0.9300
C20—C21	1.383 (4)	C46—H46	0.9300
C20—H20	0.9300	N1—N2	1.361 (2)
C21—C22	1.380 (4)	N4—N5	1.365 (3)
C21—H21	0.9300		
C6—C1—C2	120.7 (2)	C22—C23—C18	120.3 (2)
C6—C1—N1	120.6 (2)	C22—C23—H23	119.9
C2—C1—N1	118.8 (2)	C18—C23—H23	119.9
C3—C2—C1	119.0 (2)	C29—C24—C25	120.4 (2)
C3—C2—H2	120.5	C29—C24—N4	120.4 (2)
C1—C2—H2	120.5	C25—C24—N4	119.2 (2)
C4—C3—C2	121.1 (2)	C26—C25—C24	119.3 (3)
C4—C3—H3	119.5	C26—C25—H25	120.3
C2—C3—H3	119.5	C24—C25—H25	120.3
C3—C4—C5	119.6 (2)	C25—C26—C27	121.1 (3)
C3—C4—H4	120.2	C25—C26—H26	119.5
C5—C4—H4	120.2	C27—C26—H26	119.5
C4—C5—C6	120.5 (3)	C26—C27—C28	119.5 (3)
C4—C5—H5	119.7	C26—C27—H27	120.3
C6—C5—H5	119.7	C28—C27—H27	120.3
C1—C6—C5	119.2 (2)	C29—C28—C27	119.8 (3)
C1—C6—H6	120.4	C29—C28—H28	120.1
C5—C6—H6	120.4	C27—C28—H28	120.1
N2—C7—C8	110.9 (2)	C24—C29—C28	120.0 (2)
N2—C7—C10	119.2 (2)	C24—C29—H29	120.0
C8—C7—C10	129.8 (2)	C28—C29—H29	120.0
N2—C7—C10A	119.2 (2)	N5—C30—C31	111.5 (2)
C8—C7—C10A	129.8 (2)	N5—C30—C33	120.2 (2)

C9—C8—C7	103.97 (18)	C31—C30—C33	128.3 (2)
C9—C8—C14	130.5 (2)	C32—C31—C30	103.86 (18)
C7—C8—C14	125.6 (2)	C32—C31—C37	130.5 (2)
N1—C9—C8	107.7 (2)	C30—C31—C37	125.6 (2)
N1—C9—H9	126.2	N4—C32—C31	107.7 (2)
C8—C9—H9	126.2	N4—C32—H32	126.1
C11—C10—C7	127.7 (5)	C31—C32—H32	126.1
C11—C10—S1	111.5 (4)	C34—C33—C30	129.5 (2)
C7—C10—S1	120.64 (17)	C34—C33—S2	110.13 (19)
C10—C11—C12	111.1 (7)	C30—C33—S2	120.36 (17)
C10—C11—H11	124.4	C33—C34—C35	112.8 (2)
C12—C11—H11	124.4	C33—C34—H34	123.6
C13—C12—C11	112.3 (5)	C35—C34—H34	123.6
C13—C12—H12	123.9	C36—C35—C34	112.7 (3)
C11—C12—H12	123.9	C36—C35—H35	123.6
C12—C13—S1	111.9 (4)	C34—C35—H35	123.6
C12—C13—H13	124.1	C35—C36—S2	112.1 (2)
S1—C13—H13	124.1	C35—C36—H36	123.9
C13—S1—C10	93.1 (2)	S2—C36—H36	123.9
C11A—C10A—C7	120.4 (9)	C38—C37—C31	129.7 (2)
C11A—C10A—S1A	110.4 (9)	C38—C37—H37	115.2
C7—C10A—S1A	129.1 (5)	C31—C37—H37	115.2
C10A—C11A—C12A	111.9 (14)	C37—C38—C39	121.6 (2)
C10A—C11A—H11A	124.1	C37—C38—C40	123.3 (2)
C12A—C11A—H11A	124.1	C39—C38—C40	114.9 (2)
C13A—C12A—C11A	111.0 (16)	N6—C39—C38	179.2 (3)
C13A—C12A—H12A	124.5	O2—C40—C41	120.9 (2)
C11A—C12A—H12A	124.5	O2—C40—C38	118.6 (2)
C12A—C13A—S1A	111.6 (15)	C41—C40—C38	120.5 (2)
C12A—C13A—H13A	124.2	C46—C41—C42	119.3 (3)
S1A—C13A—H13A	124.2	C46—C41—C40	122.9 (2)
C10A—S1A—C13A	94.6 (9)	C42—C41—C40	117.8 (3)
C15—C14—C8	128.8 (2)	C43—C42—C41	120.3 (3)
C15—C14—H14	115.6	C43—C42—H42	119.8
C8—C14—H14	115.6	C41—C42—H42	119.8
C14—C15—C16	121.5 (2)	C42—C43—C44	120.0 (3)
C14—C15—C17	123.8 (2)	C42—C43—H43	120.0
C16—C15—C17	114.6 (2)	C44—C43—H43	120.0
N3—C16—C15	179.0 (3)	C43—C44—C45	121.2 (4)
O1—C17—C18	120.6 (2)	C43—C44—H44	119.4
O1—C17—C15	119.2 (2)	C45—C44—H44	119.4
C18—C17—C15	120.2 (2)	C46—C45—C44	118.8 (3)
C23—C18—C19	119.0 (2)	C46—C45—H45	120.6
C23—C18—C17	122.8 (2)	C44—C45—H45	120.6
C19—C18—C17	118.1 (2)	C45—C46—C41	120.3 (3)
C20—C19—C18	120.5 (3)	C45—C46—H46	119.8
C20—C19—H19	119.7	C41—C46—H46	119.8
C18—C19—H19	119.7	C9—N1—N2	112.32 (18)

C19—C20—C21	120.1 (3)	C9—N1—C1	128.2 (2)
C19—C20—H20	120.0	N2—N1—C1	119.48 (17)
C21—C20—H20	120.0	C7—N2—N1	105.10 (17)
C22—C21—C20	120.0 (3)	C32—N4—N5	112.28 (18)
C22—C21—H21	120.0	C32—N4—C24	127.8 (2)
C20—C21—H21	120.0	N5—N4—C24	119.83 (17)
C23—C22—C21	120.0 (3)	C30—N5—N4	104.61 (18)
C23—C22—H22	120.0	C36—S2—C33	92.24 (14)
C21—C22—H22	120.0		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C34—H34⋯O2[i]	0.93	2.61	3.396 (3)	143
C46—H46⋯O2[i]	0.93	2.45	3.363 (3)	167

Symmetry code: (i) $-x+1/2, y+1/2, -z+1/2$.