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N-(4-Benzoylphenyl)pyridine-2-carbothioamide

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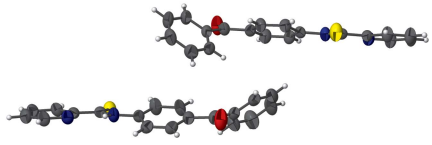
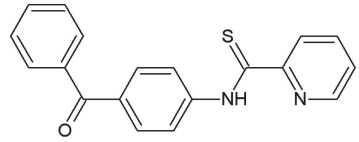
Structural data: full structural data are available from iucrdata.iucr.org

In the asymmetric unit of the title compound, $C_{19}H_{14}N_2OS$, two geometrically different molecules, *A* and *B*, are present. In *A*, the dihedral angles between the central benzene ring and pendant phenyl and pyridine groups are 56.79 (14) and 8.3 (2)°, respectively. The equivalent data for molecule *B* are 54.08 (12) and 16.7 (2)°, respectively. An intramolecular N—H···N hydrogen bond closes an *S*(5) ring in each molecule and the S and O atoms have an *anti* disposition. In the crystal, molecules are linked by a single C—H···O interaction into *A*+*B* pairs.

3D view



Chemical scheme



Structure description

Thioamides constitute an important class of compounds and, in recent years, have attracted considerable attention due to their biological activity (Meier *et al.*, 2013;Hanif *et al.*, 2014; Pagani *et al.*, 2000) as well as their applications in coordination chemistry (Meier *et al.*, 2013; Hossain *et al.*, 2004). The title compound (I) (Fig. 1) has been synthesized in the light of the above interest. The crystal structure of the related compound (4-anilinophenyl)(phenyl)methanone (Yamasaki *et al.*, 2012) has previously been published.

The title compound crystallizes with two molecules in the asymmetric unit with different conformations. One molecule (C1–C19/N1/N2/O1/S1), consists of pyridine ring *P*1 (C1–C5/N1) and benzene rings *P*2 (C7–C12) and *P*3 (C14–C19). The dihedral angles *P*1/*P*2 and *P*2/*P*3 are 8.3 (2) and 56.79 (14)°, respectively. In the second molecule (C20–C38/N3/N4/O2/S2), the constituents are the pyridine ring *P*4 (C20–C24/N3), benzene rings *P*5 (C26–C31) and *P*6 (C33–C38). In this molecule, the dihedral angles *P*4/*P*5 and *P*5/*P*6 are 16.7 (2) and 54.08 (12)°, respectively. In both molecules, an *S* (5) ring motif is present due to an intramolecular N—H···N hydrogen bond (Table 1, Fig. 2).

In the crystal, the molecules are linked into pairs by a C—H···O interaction (Table 1, Fig. 2). The pyridine ring *P*1 and the coupled benzene ring *P*2 are overlapped at a

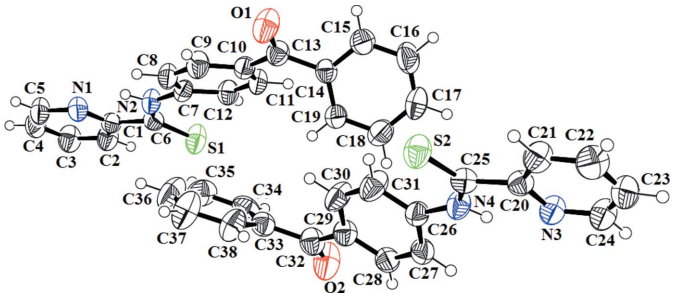


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

distance of 3.793 (2) Å due to π–π interactions with symmetry operation $(1 - x, -y, 2 - z)$.

Synthesis and crystallization

A mixture of 4-aminobenzophenone (0.986 mg, 5 mmol), sulfur (0.482 mg, 75 mmol) and sodium sulfide (0.052 mg) was refluxed in 2-picoline (10 ml) for 72 h at 413 K. After cooling the reaction mixture to room temperature, purification was carried out by passing a dichloromethane solution of the residue through a pad of silica gel. The solvent was removed and the compound was recrystallized from methanol. Light-brown needles were grown by slow evaporation of a methanol solution of the title compound.

Refinement

The studied crystal was found to be a twin with a 0.818:0.182 domain ratio. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors acknowledge the University of Sargodha for the provision of funds for the purchase of diffractometer.

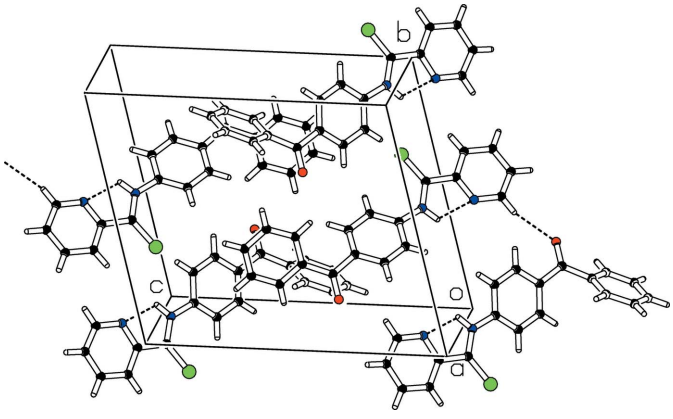


Figure 2
A partial packing (*PLATON*; Spek, 2009), showing the *S* (5) ring motif formed in individual molecules and that molecules are interlinked in pairs.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.86	2.08	2.575 (4)	116
N4—H4A···N3	0.86	2.07	2.572 (4)	116
C24—H24···O1^{i}	0.93	2.39	3.292 (5)	164

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{14}N_2OS$
M_r	318.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	9.7001 (14), 12.1805 (14), 13.8660 (17)
α, β, γ (°)	75.990 (5), 89.069 (6), 87.074 (6)
V (Å^3)	1587.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.40 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.895, 0.958
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6168, 6168, 3316
R_{int}	?
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.200, 1.00
No. of reflections	6168
No. of parameters	417
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.38

Computer programs: *APEX2* (Bruker, 2007), *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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full crystallographic data

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Crystal data

$C_{19}H_{14}N_2OS$
M_r = 318.38
Triclinic, $P\overline{1}$
a = 9.7001 (14) Å
b = 12.1805 (14) Å
c = 13.8660 (17) Å
α = 75.990 (5)°
β = 89.069 (6)°
γ = 87.074 (6)°
V = 1587.5 (4) Å^3
Z = 4
$F(000)$ = 664
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3316 reflections
θ = 1.5–26.0°
μ = 0.21 mm^{-1}
T = 296 K
Needle, light brown
0.40 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.80 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.895, T_{max} = 0.958
6168 measured reflections
6168 independent reflections
3316 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°, θ_{min} = 1.5°
h = −11→11
k = −14→15
l = −6→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.200
S = 1.00
6168 reflections
417 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0062 (19)

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	0.74371 (12)	−0.15423 (8)	0.90846 (8)	0.0690 (4)
O1	0.1987 (3)	0.3221 (2)	0.6413 (2)	0.0760 (9)
N1	0.8136 (3)	0.0431 (2)	1.0858 (2)	0.0520 (8)
N2	0.6585 (3)	0.0481 (2)	0.9357 (2)	0.0484 (7)
H2A	0.6706	0.0949	0.9719	0.058*
C1	0.8219 (3)	−0.0509 (3)	1.0526 (2)	0.0431 (8)
C2	0.9022 (4)	−0.1447 (3)	1.0968 (3)	0.0577 (10)
H2	0.9056	−0.2089	1.0716	0.069*
C3	0.9778 (4)	−0.1423 (3)	1.1793 (3)	0.0657 (11)
H3	1.0335	−0.2047	1.2108	0.079*
C4	0.9695 (4)	−0.0464 (3)	1.2140 (3)	0.0588 (10)
H4	1.0189	−0.0427	1.2699	0.071*
C5	0.8886 (4)	0.0429 (3)	1.1660 (3)	0.0595 (10)
H5	0.8847	0.1080	1.1901	0.071*
C6	0.7357 (3)	−0.0482 (3)	0.9630 (2)	0.0441 (8)
C7	0.5615 (4)	0.0880 (3)	0.8597 (2)	0.0433 (8)
C8	0.5169 (4)	0.2018 (3)	0.8436 (3)	0.0515 (9)
H8	0.5506	0.2459	0.8832	0.062*
C9	0.4243 (4)	0.2489 (3)	0.7703 (3)	0.0550 (10)
H9	0.3960	0.3249	0.7605	0.066*
C10	0.3718 (3)	0.1853 (3)	0.7100 (2)	0.0453 (8)
C11	0.4146 (4)	0.0722 (3)	0.7274 (2)	0.0479 (9)
H11	0.3801	0.0282	0.6880	0.057*
C12	0.5067 (4)	0.0230 (3)	0.8016 (3)	0.0497 (9)
H12	0.5322	−0.0537	0.8127	0.060*
C13	0.2680 (4)	0.2390 (3)	0.6332 (3)	0.0498 (9)
C14	0.2475 (4)	0.1902 (3)	0.5462 (3)	0.0440 (8)
C15	0.1162 (4)	0.1905 (3)	0.5099 (3)	0.0593 (10)
H15	0.0417	0.2181	0.5416	0.071*
C16	0.0944 (5)	0.1500 (3)	0.4268 (3)	0.0706 (12)
H16	0.0051	0.1487	0.4037	0.085*
C17	0.2036 (5)	0.1119 (3)	0.3787 (3)	0.0659 (11)
H17	0.1886	0.0852	0.3225	0.079*
C18	0.3354 (4)	0.1126 (3)	0.4126 (3)	0.0645 (11)
H18	0.4099	0.0883	0.3787	0.077*

C19	0.3567 (4)	0.1495 (3)	0.4974 (3)	0.0518 (9)
H19	0.4457	0.1471	0.5221	0.062*
S2	0.19881 (11)	0.64675 (7)	0.08840 (8)	0.0620 (3)
O2	0.7383 (3)	0.1602 (2)	0.3486 (2)	0.0839 (10)
N3	0.1800 (3)	0.4741 (2)	−0.1154 (2)	0.0533 (8)
N4	0.3075 (3)	0.4559 (2)	0.0493 (2)	0.0509 (8)
H4A	0.3048	0.4136	0.0080	0.061*
C20	0.1463 (3)	0.5547 (3)	−0.0688 (2)	0.0449 (8)
C21	0.0477 (4)	0.6404 (3)	−0.1045 (3)	0.0556 (10)
H21	0.0238	0.6944	−0.0691	0.067*
C22	−0.0139 (4)	0.6434 (3)	−0.1936 (3)	0.0649 (11)
H22	−0.0796	0.7005	−0.2202	0.078*
C23	0.0223 (4)	0.5621 (4)	−0.2424 (3)	0.0682 (11)
H23	−0.0176	0.5633	−0.3032	0.082*
C24	0.1176 (4)	0.4786 (3)	−0.2011 (3)	0.0620 (11)
H24	0.1401	0.4223	−0.2343	0.074*
C25	0.2218 (3)	0.5476 (3)	0.0266 (3)	0.0461 (9)
C26	0.4008 (4)	0.4152 (3)	0.1269 (3)	0.0466 (8)
C27	0.5035 (4)	0.3381 (3)	0.1113 (3)	0.0505 (9)
H27	0.5104	0.3203	0.0498	0.061*
C28	0.5947 (4)	0.2877 (3)	0.1844 (3)	0.0502 (9)
H28	0.6619	0.2353	0.1724	0.060*
C29	0.5882 (4)	0.3140 (3)	0.2764 (3)	0.0493 (9)
C30	0.4878 (4)	0.3913 (3)	0.2919 (3)	0.0624 (11)
H30	0.4829	0.4105	0.3528	0.075*
C31	0.3934 (4)	0.4413 (3)	0.2184 (3)	0.0669 (11)
H31	0.3250	0.4926	0.2307	0.080*
C32	0.6832 (4)	0.2501 (3)	0.3559 (3)	0.0570 (10)
C33	0.7083 (4)	0.2904 (3)	0.4468 (3)	0.0491 (9)
C34	0.7241 (4)	0.2097 (3)	0.5364 (3)	0.0606 (10)
H34	0.7180	0.1333	0.5384	0.073*
C35	0.7486 (4)	0.2429 (4)	0.6216 (3)	0.0712 (12)
H35	0.7552	0.1887	0.6816	0.085*
C36	0.7635 (5)	0.3535 (4)	0.6206 (3)	0.0840 (14)
H36	0.7816	0.3746	0.6791	0.101*
C37	0.7516 (5)	0.4336 (4)	0.5325 (3)	0.0856 (14)
H37	0.7631	0.5094	0.5309	0.103*
C38	0.7226 (4)	0.4024 (3)	0.4463 (3)	0.0664 (11)
H38	0.7126	0.4576	0.3870	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0839 (8)	0.0612 (6)	0.0699 (7)	0.0128 (5)	−0.0240 (6)	−0.0332 (5)
O1	0.095 (2)	0.0684 (17)	0.0692 (19)	0.0332 (16)	−0.0287 (16)	−0.0314 (14)
N1	0.055 (2)	0.0512 (17)	0.0528 (19)	−0.0023 (14)	−0.0099 (16)	−0.0179 (14)
N2	0.0570 (19)	0.0464 (16)	0.0447 (17)	0.0028 (14)	−0.0139 (15)	−0.0168 (13)
C1	0.042 (2)	0.048 (2)	0.039 (2)	−0.0027 (16)	−0.0015 (16)	−0.0101 (15)

C2	0.065 (3)	0.054 (2)	0.056 (2)	0.0111 (18)	−0.017 (2)	−0.0177 (18)
C3	0.067 (3)	0.065 (2)	0.065 (3)	0.015 (2)	−0.024 (2)	−0.017 (2)
C4	0.056 (3)	0.071 (3)	0.051 (2)	0.003 (2)	−0.018 (2)	−0.018 (2)
C5	0.066 (3)	0.061 (2)	0.059 (3)	0.0022 (19)	−0.018 (2)	−0.0269 (19)
C6	0.042 (2)	0.0444 (19)	0.046 (2)	−0.0039 (16)	0.0006 (17)	−0.0106 (15)
C7	0.050 (2)	0.0469 (19)	0.0362 (19)	−0.0032 (16)	−0.0002 (17)	−0.0154 (15)
C8	0.056 (2)	0.052 (2)	0.051 (2)	−0.0015 (17)	−0.0102 (19)	−0.0229 (17)
C9	0.062 (2)	0.045 (2)	0.060 (2)	0.0067 (17)	−0.013 (2)	−0.0190 (17)
C10	0.046 (2)	0.050 (2)	0.043 (2)	−0.0002 (16)	−0.0029 (17)	−0.0157 (16)
C11	0.058 (2)	0.048 (2)	0.043 (2)	0.0006 (17)	−0.0108 (18)	−0.0193 (16)
C12	0.058 (2)	0.0411 (19)	0.051 (2)	−0.0008 (16)	−0.0064 (19)	−0.0129 (16)
C13	0.054 (2)	0.050 (2)	0.045 (2)	0.0035 (18)	−0.0062 (18)	−0.0125 (17)
C14	0.045 (2)	0.0427 (18)	0.043 (2)	0.0012 (15)	−0.0075 (17)	−0.0088 (15)
C15	0.053 (3)	0.076 (3)	0.048 (2)	0.0090 (19)	−0.0094 (19)	−0.0134 (19)
C16	0.066 (3)	0.087 (3)	0.061 (3)	0.001 (2)	−0.026 (2)	−0.021 (2)
C17	0.089 (4)	0.066 (3)	0.044 (2)	−0.002 (2)	−0.017 (2)	−0.0159 (19)
C18	0.069 (3)	0.075 (3)	0.053 (3)	0.000 (2)	0.003 (2)	−0.022 (2)
C19	0.047 (2)	0.066 (2)	0.044 (2)	−0.0001 (18)	−0.0058 (18)	−0.0167 (18)
S2	0.0736 (8)	0.0532 (6)	0.0638 (7)	0.0071 (5)	−0.0109 (6)	−0.0246 (5)
O2	0.100 (2)	0.0711 (18)	0.086 (2)	0.0322 (17)	−0.0386 (19)	−0.0339 (16)
N3	0.060 (2)	0.0546 (18)	0.0479 (19)	0.0016 (15)	−0.0039 (16)	−0.0173 (14)
N4	0.058 (2)	0.0503 (17)	0.0463 (18)	0.0105 (14)	−0.0108 (16)	−0.0172 (13)
C20	0.045 (2)	0.0451 (19)	0.043 (2)	−0.0005 (16)	0.0014 (17)	−0.0090 (16)
C21	0.066 (3)	0.050 (2)	0.048 (2)	0.0036 (18)	−0.004 (2)	−0.0077 (17)
C22	0.070 (3)	0.060 (2)	0.056 (3)	0.009 (2)	−0.008 (2)	0.001 (2)
C23	0.068 (3)	0.085 (3)	0.050 (2)	−0.004 (2)	−0.010 (2)	−0.014 (2)
C24	0.072 (3)	0.066 (2)	0.051 (2)	0.000 (2)	−0.005 (2)	−0.0212 (19)
C25	0.045 (2)	0.0447 (19)	0.047 (2)	−0.0009 (16)	0.0014 (17)	−0.0085 (16)
C26	0.046 (2)	0.052 (2)	0.042 (2)	0.0006 (16)	−0.0029 (18)	−0.0133 (16)
C27	0.048 (2)	0.053 (2)	0.056 (2)	−0.0017 (17)	−0.0033 (19)	−0.0226 (18)
C28	0.044 (2)	0.049 (2)	0.061 (2)	0.0024 (16)	−0.0023 (19)	−0.0218 (18)
C29	0.050 (2)	0.0467 (19)	0.050 (2)	0.0021 (16)	−0.0063 (18)	−0.0110 (17)
C30	0.077 (3)	0.073 (2)	0.038 (2)	0.023 (2)	−0.009 (2)	−0.0190 (18)
C31	0.077 (3)	0.074 (3)	0.052 (2)	0.030 (2)	−0.009 (2)	−0.025 (2)
C32	0.057 (2)	0.054 (2)	0.060 (3)	0.0020 (18)	−0.009 (2)	−0.0140 (18)
C33	0.044 (2)	0.051 (2)	0.052 (2)	0.0029 (16)	−0.0054 (18)	−0.0120 (18)
C34	0.043 (2)	0.066 (2)	0.066 (3)	−0.0008 (18)	−0.007 (2)	−0.004 (2)
C35	0.064 (3)	0.094 (3)	0.048 (3)	0.009 (2)	−0.003 (2)	−0.004 (2)
C36	0.104 (4)	0.105 (4)	0.047 (3)	0.020 (3)	−0.012 (3)	−0.030 (3)
C37	0.129 (4)	0.069 (3)	0.064 (3)	0.009 (3)	−0.013 (3)	−0.027 (2)
C38	0.097 (3)	0.055 (2)	0.047 (2)	0.002 (2)	−0.005 (2)	−0.0127 (18)

Geometric parameters (Å, º)

S1—C6	1.644 (3)	S2—C25	1.646 (3)
O1—C13	1.214 (4)	O2—C32	1.218 (4)
N1—C1	1.333 (4)	N3—C20	1.325 (4)
N1—C5	1.338 (4)	N3—C24	1.330 (4)

N2—C6	1.336 (4)	N4—C25	1.334 (4)
N2—C7	1.403 (4)	N4—C26	1.396 (4)
N2—H2A	0.8600	N4—H4A	0.8600
C1—C2	1.368 (5)	C20—C21	1.382 (5)
C1—C6	1.503 (5)	C20—C25	1.504 (5)
C2—C3	1.376 (5)	C21—C22	1.373 (5)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.364 (5)	C22—C23	1.357 (5)
C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.350 (5)	C23—C24	1.362 (5)
C4—H4	0.9300	C23—H23	0.9300
C5—H5	0.9300	C24—H24	0.9300
C7—C12	1.388 (4)	C26—C31	1.381 (5)
C7—C8	1.396 (4)	C26—C27	1.385 (5)
C8—C9	1.365 (5)	C27—C28	1.363 (5)
C8—H8	0.9300	C27—H27	0.9300
C9—C10	1.389 (4)	C28—C29	1.388 (5)
C9—H9	0.9300	C28—H28	0.9300
C10—C11	1.382 (4)	C29—C30	1.371 (5)
C10—C13	1.485 (5)	C29—C32	1.488 (5)
C11—C12	1.375 (5)	C30—C31	1.386 (5)
C11—H11	0.9300	C30—H30	0.9300
C12—H12	0.9300	C31—H31	0.9300
C13—C14	1.488 (5)	C32—C33	1.487 (5)
C14—C15	1.376 (5)	C33—C38	1.376 (5)
C14—C19	1.382 (5)	C33—C34	1.391 (5)
C15—C16	1.382 (5)	C34—C35	1.366 (5)
C15—H15	0.9300	C34—H34	0.9300
C16—C17	1.364 (6)	C35—C36	1.359 (6)
C16—H16	0.9300	C35—H35	0.9300
C17—C18	1.371 (6)	C36—C37	1.369 (6)
C17—H17	0.9300	C36—H36	0.9300
C18—C19	1.379 (5)	C37—C38	1.377 (5)
C18—H18	0.9300	C37—H37	0.9300
C19—H19	0.9300	C38—H38	0.9300
C1—N1—C5	116.8 (3)	C20—N3—C24	117.8 (3)
C6—N2—C7	132.8 (3)	C25—N4—C26	132.7 (3)
C6—N2—H2A	113.6	C25—N4—H4A	113.7
C7—N2—H2A	113.6	C26—N4—H4A	113.7
N1—C1—C2	122.9 (3)	N3—C20—C21	122.7 (3)
N1—C1—C6	115.5 (3)	N3—C20—C25	115.9 (3)
C2—C1—C6	121.6 (3)	C21—C20—C25	121.4 (3)
C1—C2—C3	118.8 (3)	C22—C21—C20	118.2 (4)
C1—C2—H2	120.6	C22—C21—H21	120.9
C3—C2—H2	120.6	C20—C21—H21	120.9
C4—C3—C2	118.6 (4)	C23—C22—C21	119.2 (4)
C4—C3—H3	120.7	C23—C22—H22	120.4

C2—C3—H3	120.7	C21—C22—H22	120.4
C5—C4—C3	119.1 (3)	C22—C23—C24	119.2 (4)
C5—C4—H4	120.4	C22—C23—H23	120.4
C3—C4—H4	120.4	C24—C23—H23	120.4
N1—C5—C4	123.7 (3)	N3—C24—C23	122.9 (4)
N1—C5—H5	118.2	N3—C24—H24	118.5
C4—C5—H5	118.2	C23—C24—H24	118.5
N2—C6—C1	111.9 (3)	N4—C25—C20	111.5 (3)
N2—C6—S1	127.0 (3)	N4—C25—S2	127.3 (3)
C1—C6—S1	121.2 (2)	C20—C25—S2	121.3 (2)
C12—C7—C8	118.6 (3)	C31—C26—C27	118.4 (3)
C12—C7—N2	125.0 (3)	C31—C26—N4	125.0 (3)
C8—C7—N2	116.4 (3)	C27—C26—N4	116.5 (3)
C9—C8—C7	120.8 (3)	C28—C27—C26	121.2 (3)
C9—C8—H8	119.6	C28—C27—H27	119.4
C7—C8—H8	119.6	C26—C27—H27	119.4
C8—C9—C10	121.0 (3)	C27—C28—C29	120.7 (3)
C8—C9—H9	119.5	C27—C28—H28	119.7
C10—C9—H9	119.5	C29—C28—H28	119.7
C11—C10—C9	118.0 (3)	C30—C29—C28	118.3 (3)
C11—C10—C13	122.7 (3)	C30—C29—C32	123.1 (3)
C9—C10—C13	119.3 (3)	C28—C29—C32	118.3 (3)
C12—C11—C10	121.8 (3)	C29—C30—C31	121.3 (3)
C12—C11—H11	119.1	C29—C30—H30	119.4
C10—C11—H11	119.1	C31—C30—H30	119.4
C11—C12—C7	119.9 (3)	C26—C31—C30	120.1 (3)
C11—C12—H12	120.1	C26—C31—H31	120.0
C7—C12—H12	120.1	C30—C31—H31	120.0
O1—C13—C10	120.3 (3)	O2—C32—C33	118.7 (3)
O1—C13—C14	119.6 (3)	O2—C32—C29	119.6 (3)
C10—C13—C14	120.0 (3)	C33—C32—C29	121.6 (3)
C15—C14—C19	118.7 (3)	C38—C33—C34	118.4 (4)
C15—C14—C13	119.0 (3)	C38—C33—C32	123.7 (3)
C19—C14—C13	122.2 (3)	C34—C33—C32	117.9 (3)
C14—C15—C16	120.5 (4)	C35—C34—C33	119.9 (4)
C14—C15—H15	119.8	C35—C34—H34	120.1
C16—C15—H15	119.8	C33—C34—H34	120.1
C17—C16—C15	120.0 (4)	C36—C35—C34	121.4 (4)
C17—C16—H16	120.0	C36—C35—H35	119.3
C15—C16—H16	120.0	C34—C35—H35	119.3
C16—C17—C18	120.5 (4)	C35—C36—C37	119.3 (4)
C16—C17—H17	119.8	C35—C36—H36	120.3
C18—C17—H17	119.8	C37—C36—H36	120.3
C17—C18—C19	119.5 (4)	C36—C37—C38	120.2 (4)
C17—C18—H18	120.3	C36—C37—H37	119.9
C19—C18—H18	120.3	C38—C37—H37	119.9
C18—C19—C14	120.8 (3)	C33—C38—C37	120.7 (4)
C18—C19—H19	119.6	C33—C38—H38	119.6

C14—C19—H19	119.6	C37—C38—H38	119.6
C5—N1—C1—C2	0.0 (5)	C24—N3—C20—C21	1.5 (5)
C5—N1—C1—C6	179.5 (3)	C24—N3—C20—C25	−178.7 (3)
N1—C1—C2—C3	0.1 (6)	N3—C20—C21—C22	−2.1 (5)
C6—C1—C2—C3	−179.4 (3)	C25—C20—C21—C22	178.1 (3)
C1—C2—C3—C4	0.2 (6)	C20—C21—C22—C23	0.9 (6)
C2—C3—C4—C5	−0.5 (6)	C21—C22—C23—C24	0.8 (6)
C1—N1—C5—C4	−0.4 (6)	C20—N3—C24—C23	0.3 (6)
C3—C4—C5—N1	0.7 (6)	C22—C23—C24—N3	−1.5 (6)
C7—N2—C6—C1	−178.5 (3)	C26—N4—C25—C20	177.8 (3)
C7—N2—C6—S1	2.5 (6)	C26—N4—C25—S2	−0.2 (6)
N1—C1—C6—N2	−3.7 (4)	N3—C20—C25—N4	−2.5 (4)
C2—C1—C6—N2	175.8 (3)	C21—C20—C25—N4	177.3 (3)
N1—C1—C6—S1	175.4 (2)	N3—C20—C25—S2	175.5 (3)
C2—C1—C6—S1	−5.1 (5)	C21—C20—C25—S2	−4.6 (5)
C6—N2—C7—C12	11.0 (6)	C25—N4—C26—C31	23.5 (6)
C6—N2—C7—C8	−169.9 (4)	C25—N4—C26—C27	−160.1 (3)
C12—C7—C8—C9	−1.9 (5)	C31—C26—C27—C28	0.7 (5)
N2—C7—C8—C9	179.0 (3)	N4—C26—C27—C28	−175.9 (3)
C7—C8—C9—C10	0.2 (6)	C26—C27—C28—C29	−1.0 (5)
C8—C9—C10—C11	0.9 (5)	C27—C28—C29—C30	0.2 (5)
C8—C9—C10—C13	178.1 (3)	C27—C28—C29—C32	175.3 (3)
C9—C10—C11—C12	−0.3 (5)	C28—C29—C30—C31	0.9 (6)
C13—C10—C11—C12	−177.4 (3)	C32—C29—C30—C31	−174.1 (4)
C10—C11—C12—C7	−1.4 (5)	C27—C26—C31—C30	0.3 (6)
C8—C7—C12—C11	2.5 (5)	N4—C26—C31—C30	176.7 (3)
N2—C7—C12—C11	−178.4 (3)	C29—C30—C31—C26	−1.1 (6)
C11—C10—C13—O1	154.4 (4)	C30—C29—C32—O2	156.8 (4)
C9—C10—C13—O1	−22.6 (5)	C28—C29—C32—O2	−18.1 (5)
C11—C10—C13—C14	−24.9 (5)	C30—C29—C32—C33	−20.5 (6)
C9—C10—C13—C14	158.1 (3)	C28—C29—C32—C33	164.6 (3)
O1—C13—C14—C15	−36.6 (5)	O2—C32—C33—C38	142.6 (4)
C10—C13—C14—C15	142.6 (3)	C29—C32—C33—C38	−40.1 (5)
O1—C13—C14—C19	140.1 (4)	O2—C32—C33—C34	−34.4 (5)
C10—C13—C14—C19	−40.6 (5)	C29—C32—C33—C34	142.8 (4)
C19—C14—C15—C16	0.5 (5)	C38—C33—C34—C35	2.2 (6)
C13—C14—C15—C16	177.4 (3)	C32—C33—C34—C35	179.4 (4)
C14—C15—C16—C17	−1.6 (6)	C33—C34—C35—C36	−2.7 (6)
C15—C16—C17—C18	0.5 (6)	C34—C35—C36—C37	1.0 (7)
C16—C17—C18—C19	1.6 (6)	C35—C36—C37—C38	1.0 (8)
C17—C18—C19—C14	−2.7 (6)	C34—C33—C38—C37	−0.1 (6)
C15—C14—C19—C18	1.6 (5)	C32—C33—C38—C37	−177.2 (4)
C13—C14—C19—C18	−175.2 (3)	C36—C37—C38—C33	−1.5 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N1	0.86	2.08	2.575 (4)	116
N4—H4*A*···N3	0.86	2.07	2.572 (4)	116
C24—H24···O1^{i}	0.93	2.39	3.292 (5)	164

Symmetry code: (i) *x*, *y*, *z*−1.