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2,6-Bis(1-isopropyl-5-phenyl-1*H*-pyrazol-3-yl)pyridine

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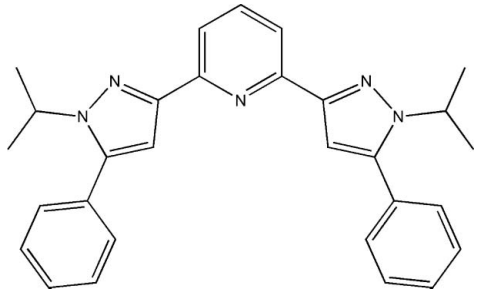
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.123; data-to-parameter ratio = 14.1.

In the title compound, $C_{29}H_{29}N_5$, the central pyridine ring and the two pyrazole rings are approximately coplanar, the dihedral angles between the pyridine and pyrazole rings being 3.94 (12) and 14.84 (12)°. The pyrazole and phenyl rings on each side of the molecule are twisted with dihedral angles of 46.72 (8) and 73.39 (8)°. One phenyl ring interacts with a pyrazole ring of a neighbouring molecule *via* a weak intermolecular C—H$\cdots\pi$ interaction, which stabilizes the molecular packing.

Related literature

For general background, see: Dias & Gamage (2007); Zhou & Chen (2007).



Experimental

Crystal data

$C_{29}H_{29}N_5$
M_r = 447.57
Triclinic, $P\overline{1}$
a = 9.973 (3) Å
b = 10.172 (3) Å
c = 14.014 (4) Å
α = 110.940 (4)°
β = 106.494 (4)°
γ = 94.583 (4)°
V = 1246.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.53 × 0.43 × 0.39 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.963, T_{max} = 0.972
6572 measured reflections
4332 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.05
4332 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C20—H20$\cdots Cg1^{i}$	0.93	2.86	3.710 (3)	153

Symmetry code: (i) $-x+1, -y, -z$. $Cg1$ is the centroid of the C6-C8/N2/N3 pyrazole ring.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2264).

References

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Zhou, Y. B. & Chen, W. Z. (2007). *Dalton Trans.* pp. 5123–5125.

supporting information

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2,6-Bis(1-isopropyl-5-phenyl-1*H*-pyrazol-3-yl)pyridine

Ping Liu, Yong-Bo Zhou, Min-Guo Li and Cai-Xia An

S1. Comment

Pyrazolyl ligands are a kind of mutifuntional organic ligands often displaying *exo*-bidentate coordination mode (Dias & Gamage, 2007). The title compound, 2,6-bis(5-phenyl-1-isopropyl-1*H*-pyrazol-3-yl)pyridine (hereinafter abbreviated to bpipp), is a potentially tridentate pincer ligand by *N*-alkylation of a bispyrazolyl ligand.

The asymmetric unit of the title compound contains only one bpipp molecule (Fig. 1). The pyrazole and pyridine rings are near-coplanar [inter-ring dihedral angles 3.94 (12) and 14.84 (12)°], whereas the pyrazole rings are twisted from the phenyl rings with the two dihedral angles 46.72 (8) and 73.39 (8)°. The phenyl ring interacts with the pyrazole ring of the neighbouring molecule to afford a weak intermolecular C—H··· π interaction (Table 1; *Cg*1 is the centroid of the C6—C8/N2/N3 pyrazole ring) which stabilizes the molecular packing. The centroid to centroid distance between stacked pyridine rings is *ca* 4.88 Å, which is very long and prevents π-π stacking (Fig. 2). All bond lengths and angles are normal.

S2. Experimental

All chemicals were of reagent grade quality obtained from commercial sources and used as received, unless stated otherwise. 2,6-bis(5-phenyl-1*H*-pyrazol-3-yl)pyridine (bppp) was prepared by the general procedure of Zhou and Chen (2007). A mixture of bppp (0.72 g, 2 mmol) and 60% NaH (0.32 g, 8 mmol) in dry DMF (15 ml) was stirred for 2 h at room temperature. To the solution was added 2-bromopropane (0.98 g, 8 mmol). After stirring at 333 K for two days, the resulting solution was concentrated to 4 ml. Addition of H_2O (15 ml) precipitated a pale yellow powder. Column chromatography involved elution with ethyl acetate/ petroleum ether (1:4) separated the compound as a white powder (0.56 g). Yield: 62%. Anal. Calcd for $C_{29}H_{29}N_5$: C 77.82, H 6.53, N 15.65; Found: C 77.60, H 6.62, N 15.57. MS (*m*/*z*): 447 (M^+, 100), 432, 405, 390, 363, 334, 304, 195, 168, 115, 77. ^{1}H NMR (DMSO-d_6): 7.90 (br, 3H), 7.56–7.48 (m, 10H), 6.99 (s, 2H), 4.58(m, 2H), 1.47(s, 6H), 1.45 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 151.8, 150.5, 144.5, 130.6, 129.3, 129.2, 129.0, 125.14, 118.1, 104.8, 50.3, 23.2, 23.1. Colorless single crystals were grown from slow evaporation of a saturated MeOH solution of the compound.

S3. Refinement

H atoms were positioned geometrically and treated as riding, with C—H bonding lengths constrained to 0.93 (aromatic CH), 0.98 (methylene CH), or 0.96 Å (methyl CH_3), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

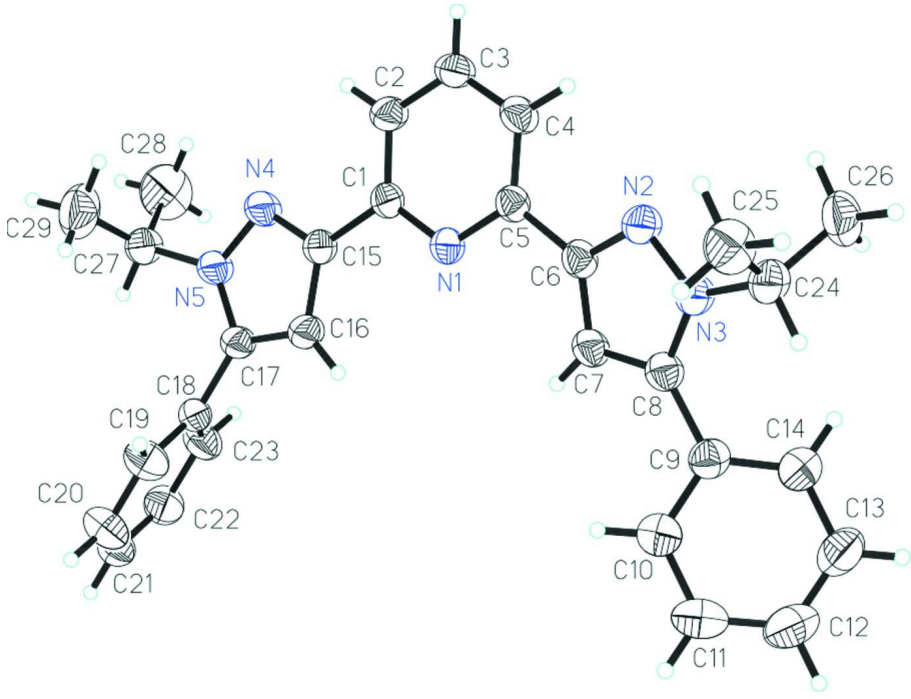

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

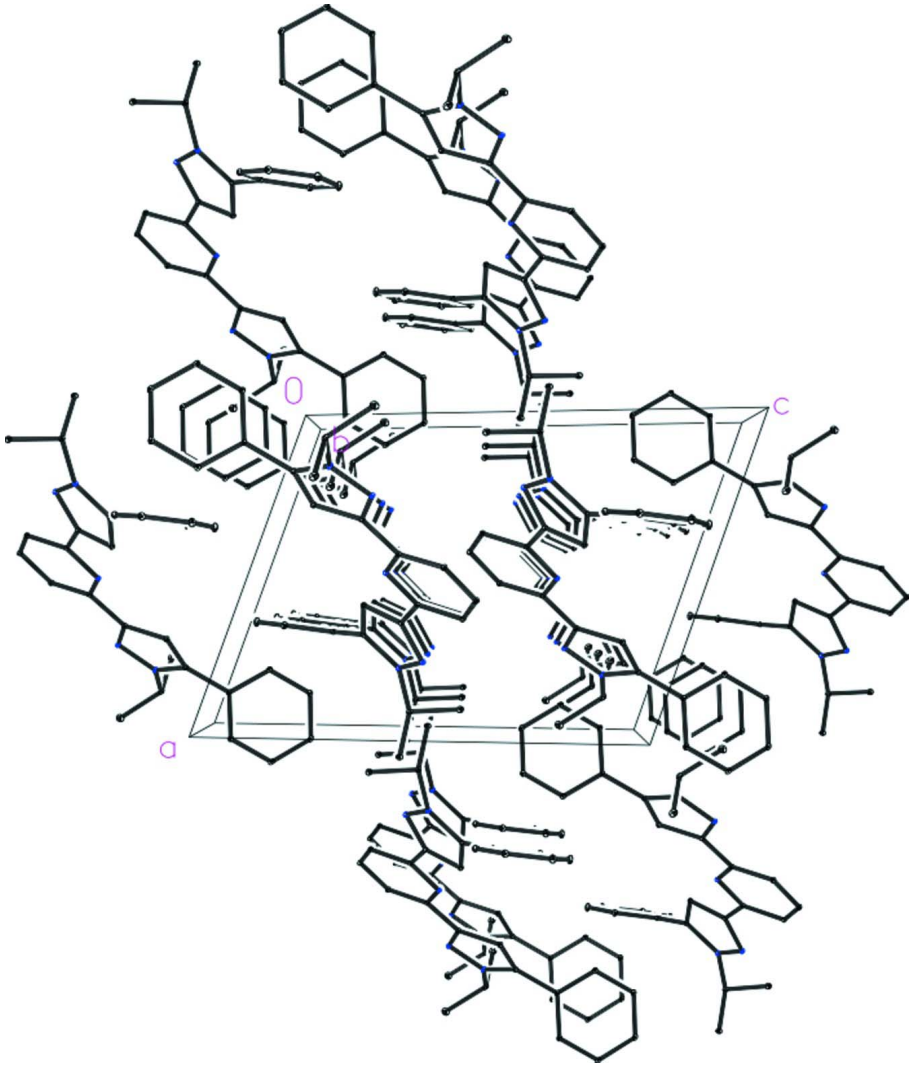

Figure 2

A packing view of the title compound along the *b* axis. H atoms have been omitted for clarity.

2,6-Bis(1-isopropyl-5-phenyl-1*H*-pyrazol-3-yl)pyridine

Crystal data

$C_{29}H_{29}N_5$
$M_r = 447.57$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.973\ (3)$ Å
$b = 10.172\ (3)$ Å
$c = 14.014\ (4)$ Å
$\alpha = 110.940\ (4)°$
$\beta = 106.494\ (4)°$
$\gamma = 94.583\ (4)°$
$V = 1246.8\ (6)$ Å^3
$Z = 2$
$F(000) = 476$
$D_x = 1.192$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1546 reflections
$\theta = 2.8–21.8°$
$\mu = 0.07$ mm^{-1}
$T = 298$ K
Prism, colorless
0.53 × 0.43 × 0.39 mm

Data collection

SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.963, T_{max} = 0.972
6572 measured reflections
4332 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 2.2°
$h = -11 \rightarrow 7$
$k = -10 \rightarrow 12$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.05
4332 reflections
307 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
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.0355P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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^ > σ(*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}
N1	0.49140 (17)	0.25670 (17)	0.32171 (13)	0.0437 (5)
N2	0.75204 (19)	0.58665 (18)	0.45974 (14)	0.0507 (5)
N3	0.77219 (19)	0.67986 (18)	0.41370 (14)	0.0510 (5)
N4	0.28141 (19)	−0.09220 (18)	0.24676 (14)	0.0522 (5)
N5	0.19993 (19)	−0.17780 (17)	0.14410 (14)	0.0519 (5)
C1	0.4400 (2)	0.1424 (2)	0.33672 (17)	0.0419 (5)
C2	0.4774 (2)	0.1347 (2)	0.43729 (17)	0.0494 (6)
H2	0.4400	0.0539	0.4450	0.059*
C3	0.5705 (2)	0.2481 (2)	0.52506 (18)	0.0520 (6)
H3	0.5976	0.2451	0.5933	0.062*
C4	0.6235 (2)	0.3662 (2)	0.51153 (17)	0.0491 (6)
H4	0.6857	0.4449	0.5705	0.059*
C5	0.5832 (2)	0.3665 (2)	0.40889 (17)	0.0412 (5)
C6	0.6374 (2)	0.4876 (2)	0.38672 (17)	0.0437 (5)
C7	0.5864 (2)	0.5158 (2)	0.29458 (17)	0.0473 (6)

H7	0.5088	0.4614	0.2327	0.057*
C8	0.6735 (2)	0.6402 (2)	0.31321 (18)	0.0468 (6)
C9	0.6679 (2)	0.7231 (2)	0.24527 (19)	0.0492 (6)
C10	0.6480 (3)	0.6519 (3)	0.1365 (2)	0.0699 (8)
H10	0.6402	0.5528	0.1073	0.084*
C11	0.6396 (3)	0.7265 (4)	0.0706 (2)	0.0927 (10)
H11	0.6257	0.6775	−0.0027	0.111*
C12	0.6517 (3)	0.8726 (4)	0.1130 (3)	0.0894 (9)
H12	0.6478	0.9227	0.0687	0.107*
C13	0.6693 (3)	0.9441 (3)	0.2190 (3)	0.0743 (8)
H13	0.6771	1.0433	0.2475	0.089*
C14	0.6757 (3)	0.8699 (3)	0.2845 (2)	0.0623 (7)
H14	0.6856	0.9196	0.3569	0.075*
C15	0.3432 (2)	0.0234 (2)	0.23969 (17)	0.0436 (5)
C16	0.3022 (2)	0.0097 (2)	0.13208 (17)	0.0489 (6)
H16	0.3311	0.0759	0.1065	0.059*
C17	0.2110 (2)	−0.1202 (2)	0.07220 (16)	0.0454 (6)
C18	0.1321 (3)	−0.1941 (2)	−0.04508 (17)	0.0469 (6)
C19	0.2024 (3)	−0.2537 (3)	−0.1166 (2)	0.0655 (7)
H19	0.3005	−0.2471	−0.0907	0.079*
C20	0.1282 (3)	−0.3234 (3)	−0.2265 (2)	0.0724 (8)
H20	0.1766	−0.3643	−0.2740	0.087*
C21	−0.0148 (3)	−0.3324 (2)	−0.2656 (2)	0.0632 (7)
H21	−0.0641	−0.3793	−0.3397	0.076*
C22	−0.0861 (3)	−0.2729 (3)	−0.1964 (2)	0.0647 (7)
H22	−0.1841	−0.2792	−0.2230	0.078*
C23	−0.0128 (3)	−0.2035 (2)	−0.08679 (19)	0.0603 (7)
H23	−0.0620	−0.1621	−0.0401	0.072*
C24	0.9034 (2)	0.7923 (2)	0.46856 (19)	0.0549 (6)
H24	0.9062	0.8436	0.4216	0.066*
C25	1.0336 (3)	0.7258 (3)	0.4818 (2)	0.0694 (7)
H25A	1.0305	0.6584	0.4122	0.104*
H25B	1.0354	0.6768	0.5292	0.104*
H25C	1.1180	0.7998	0.5123	0.104*
C26	0.8991 (3)	0.8999 (2)	0.5743 (2)	0.0707 (8)
H26A	0.8147	0.9392	0.5609	0.106*
H26B	0.9820	0.9759	0.6067	0.106*
H26C	0.8978	0.8530	0.6227	0.106*
C27	0.1273 (3)	−0.3221 (2)	0.12085 (19)	0.0606 (7)
H27	0.0613	−0.3627	0.0459	0.073*
C28	0.0417 (3)	−0.3145 (3)	0.1945 (3)	0.1074 (11)
H28A	−0.0257	−0.2539	0.1854	0.161*
H28B	0.1046	−0.2755	0.2684	0.161*
H28C	−0.0085	−0.4093	0.1766	0.161*
C29	0.2353 (3)	−0.4163 (3)	0.1301 (2)	0.0955 (10)
H29A	0.2869	−0.4181	0.0815	0.143*
H29B	0.1870	−0.5121	0.1116	0.143*
H29C	0.3007	−0.3787	0.2032	0.143*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0443 (11)	0.0382 (10)	0.0421 (11)	−0.0014 (9)	0.0103 (9)	0.0141 (9)
N2	0.0509 (12)	0.0475 (11)	0.0481 (11)	−0.0066 (9)	0.0097 (10)	0.0214 (9)
N3	0.0506 (12)	0.0459 (11)	0.0497 (12)	−0.0065 (9)	0.0095 (10)	0.0205 (9)
N4	0.0565 (12)	0.0441 (11)	0.0403 (11)	−0.0105 (9)	0.0036 (9)	0.0132 (9)
N5	0.0594 (13)	0.0424 (11)	0.0393 (11)	−0.0091 (9)	0.0037 (10)	0.0137 (9)
C1	0.0401 (13)	0.0374 (12)	0.0413 (13)	0.0013 (10)	0.0089 (10)	0.0131 (10)
C2	0.0519 (14)	0.0473 (13)	0.0439 (14)	−0.0016 (11)	0.0075 (12)	0.0214 (11)
C3	0.0570 (15)	0.0535 (14)	0.0390 (13)	−0.0010 (12)	0.0081 (12)	0.0197 (11)
C4	0.0458 (14)	0.0482 (14)	0.0410 (14)	−0.0025 (11)	0.0067 (11)	0.0124 (11)
C5	0.0390 (12)	0.0383 (12)	0.0410 (13)	0.0022 (10)	0.0116 (10)	0.0124 (10)
C6	0.0414 (13)	0.0403 (12)	0.0429 (14)	0.0002 (10)	0.0125 (11)	0.0123 (10)
C7	0.0460 (14)	0.0445 (13)	0.0404 (13)	−0.0023 (11)	0.0077 (11)	0.0121 (11)
C8	0.0447 (14)	0.0465 (13)	0.0443 (14)	0.0037 (11)	0.0114 (11)	0.0166 (11)
C9	0.0435 (14)	0.0525 (14)	0.0516 (15)	0.0037 (11)	0.0138 (11)	0.0239 (12)
C10	0.091 (2)	0.0616 (16)	0.0548 (17)	0.0085 (15)	0.0238 (15)	0.0228 (14)
C11	0.132 (3)	0.098 (2)	0.0558 (19)	0.021 (2)	0.0343 (18)	0.0376 (18)
C12	0.120 (3)	0.090 (2)	0.084 (2)	0.027 (2)	0.042 (2)	0.057 (2)
C13	0.090 (2)	0.0635 (17)	0.088 (2)	0.0216 (15)	0.0353 (18)	0.0445 (17)
C14	0.0726 (18)	0.0569 (16)	0.0619 (17)	0.0134 (13)	0.0242 (14)	0.0274 (14)
C15	0.0450 (13)	0.0386 (12)	0.0415 (13)	−0.0004 (10)	0.0093 (11)	0.0154 (10)
C16	0.0562 (15)	0.0434 (13)	0.0432 (14)	−0.0009 (11)	0.0111 (11)	0.0195 (11)
C17	0.0489 (14)	0.0437 (13)	0.0372 (13)	0.0027 (11)	0.0072 (11)	0.0157 (11)
C18	0.0556 (15)	0.0380 (12)	0.0382 (13)	0.0017 (11)	0.0077 (12)	0.0131 (10)
C19	0.0613 (17)	0.0722 (17)	0.0494 (17)	0.0066 (14)	0.0105 (14)	0.0167 (14)
C20	0.079 (2)	0.0789 (19)	0.0476 (17)	0.0149 (16)	0.0219 (15)	0.0116 (14)
C21	0.082 (2)	0.0518 (15)	0.0399 (15)	0.0044 (14)	0.0058 (15)	0.0136 (12)
C22	0.0591 (17)	0.0623 (16)	0.0521 (17)	0.0051 (13)	−0.0022 (14)	0.0172 (13)
C23	0.0582 (17)	0.0623 (16)	0.0450 (15)	0.0106 (13)	0.0088 (13)	0.0110 (12)
C24	0.0507 (15)	0.0502 (14)	0.0573 (16)	−0.0097 (12)	0.0108 (12)	0.0239 (12)
C25	0.0542 (17)	0.0721 (17)	0.0763 (19)	0.0010 (14)	0.0205 (14)	0.0266 (14)
C26	0.0722 (18)	0.0486 (15)	0.0715 (18)	−0.0080 (13)	0.0199 (15)	0.0092 (13)
C27	0.0692 (17)	0.0422 (14)	0.0496 (15)	−0.0176 (13)	−0.0001 (13)	0.0164 (12)
C28	0.107 (3)	0.091 (2)	0.120 (3)	−0.0275 (19)	0.048 (2)	0.038 (2)
C29	0.106 (2)	0.0529 (17)	0.105 (3)	0.0048 (17)	0.016 (2)	0.0243 (16)

Geometric parameters (Å, º)

N1—C1	1.341 (2)	C15—C16	1.397 (3)
N1—C5	1.343 (2)	C16—C17	1.364 (3)
N2—C6	1.335 (2)	C16—H16	0.9300
N2—N3	1.355 (2)	C17—C18	1.474 (3)
N3—C8	1.363 (2)	C18—C19	1.377 (3)
N3—C24	1.474 (2)	C18—C23	1.378 (3)
N4—C15	1.332 (2)	C19—C20	1.383 (3)
N4—N5	1.348 (2)	C19—H19	0.9300

N5—C17	1.358 (3)	C20—C21	1.357 (3)
N5—C27	1.463 (2)	C20—H20	0.9300
C1—C2	1.385 (3)	C21—C22	1.362 (3)
C1—C15	1.462 (3)	C21—H21	0.9300
C2—C3	1.368 (3)	C22—C23	1.377 (3)
C2—H2	0.9300	C22—H22	0.9300
C3—C4	1.370 (3)	C23—H23	0.9300
C3—H3	0.9300	C24—C25	1.507 (3)
C4—C5	1.380 (3)	C24—C26	1.510 (3)
C4—H4	0.9300	C24—H24	0.9800
C5—C6	1.473 (3)	C25—H25A	0.9600
C6—C7	1.387 (3)	C25—H25B	0.9600
C7—C8	1.373 (3)	C25—H25C	0.9600
C7—H7	0.9300	C26—H26A	0.9600
C8—C9	1.474 (3)	C26—H26B	0.9600
C9—C10	1.380 (3)	C26—H26C	0.9600
C9—C14	1.381 (3)	C27—C28	1.501 (4)
C10—C11	1.378 (3)	C27—C29	1.506 (3)
C10—H10	0.9300	C27—H27	0.9800
C11—C12	1.369 (4)	C28—H28A	0.9600
C11—H11	0.9300	C28—H28B	0.9600
C12—C13	1.351 (4)	C28—H28C	0.9600
C12—H12	0.9300	C29—H29A	0.9600
C13—C14	1.374 (3)	C29—H29B	0.9600
C13—H13	0.9300	C29—H29C	0.9600
C14—H14	0.9300		

C1—N1—C5	117.55 (18)	N5—C17—C16	105.95 (18)
C6—N2—N3	104.67 (17)	N5—C17—C18	122.37 (18)
N2—N3—C8	112.07 (16)	C16—C17—C18	131.7 (2)
N2—N3—C24	117.84 (17)	C19—C18—C23	118.0 (2)
C8—N3—C24	129.40 (18)	C19—C18—C17	120.6 (2)
C15—N4—N5	104.86 (17)	C23—C18—C17	121.5 (2)
N4—N5—C17	112.34 (16)	C18—C19—C20	120.6 (2)
N4—N5—C27	119.23 (17)	C18—C19—H19	119.7
C17—N5—C27	127.95 (18)	C20—C19—H19	119.7
N1—C1—C2	122.68 (18)	C21—C20—C19	120.4 (3)
N1—C1—C15	116.11 (18)	C21—C20—H20	119.8
C2—C1—C15	121.20 (18)	C19—C20—H20	119.8
C3—C2—C1	118.8 (2)	C20—C21—C22	120.0 (2)
C3—C2—H2	120.6	C20—C21—H21	120.0
C1—C2—H2	120.6	C22—C21—H21	120.0
C2—C3—C4	119.5 (2)	C21—C22—C23	119.9 (2)
C2—C3—H3	120.3	C21—C22—H22	120.1
C4—C3—H3	120.3	C23—C22—H22	120.1
C3—C4—C5	118.91 (19)	C22—C23—C18	121.2 (3)
C3—C4—H4	120.5	C22—C23—H23	119.4
C5—C4—H4	120.5	C18—C23—H23	119.4

N1—C5—C4	122.63 (18)	N3—C24—C25	110.52 (18)
N1—C5—C6	114.89 (18)	N3—C24—C26	110.4 (2)
C4—C5—C6	122.47 (18)	C25—C24—C26	113.2 (2)
N2—C6—C7	111.30 (18)	N3—C24—H24	107.5
N2—C6—C5	120.23 (19)	C25—C24—H24	107.5
C7—C6—C5	128.46 (19)	C26—C24—H24	107.5
C8—C7—C6	106.11 (18)	C24—C25—H25A	109.5
C8—C7—H7	126.9	C24—C25—H25B	109.5
C6—C7—H7	126.9	H25A—C25—H25B	109.5
N3—C8—C7	105.83 (18)	C24—C25—H25C	109.5
N3—C8—C9	123.87 (18)	H25A—C25—H25C	109.5
C7—C8—C9	130.3 (2)	H25B—C25—H25C	109.5
C10—C9—C14	117.7 (2)	C24—C26—H26A	109.5
C10—C9—C8	119.4 (2)	C24—C26—H26B	109.5
C14—C9—C8	122.9 (2)	H26A—C26—H26B	109.5
C11—C10—C9	120.6 (3)	C24—C26—H26C	109.5
C11—C10—H10	119.7	H26A—C26—H26C	109.5
C9—C10—H10	119.7	H26B—C26—H26C	109.5
C12—C11—C10	120.1 (3)	N5—C27—C28	110.2 (2)
C12—C11—H11	120.0	N5—C27—C29	109.6 (2)
C10—C11—H11	120.0	C28—C27—C29	112.5 (2)
C13—C12—C11	120.3 (3)	N5—C27—H27	108.2
C13—C12—H12	119.8	C28—C27—H27	108.2
C11—C12—H12	119.8	C29—C27—H27	108.2
C12—C13—C14	119.7 (3)	C27—C28—H28A	109.5
C12—C13—H13	120.1	C27—C28—H28B	109.5
C14—C13—H13	120.1	H28A—C28—H28B	109.5
C13—C14—C9	121.5 (2)	C27—C28—H28C	109.5
C13—C14—H14	119.2	H28A—C28—H28C	109.5
C9—C14—H14	119.2	H28B—C28—H28C	109.5
N4—C15—C16	110.78 (18)	C27—C29—H29A	109.5
N4—C15—C1	120.71 (19)	C27—C29—H29B	109.5
C16—C15—C1	128.51 (19)	H29A—C29—H29B	109.5
C17—C16—C15	106.06 (18)	C27—C29—H29C	109.5
C17—C16—H16	127.0	H29A—C29—H29C	109.5
C15—C16—H16	127.0	H29B—C29—H29C	109.5

C6—N2—N3—C8	−0.6 (2)	C12—C13—C14—C9	1.5 (4)
C6—N2—N3—C24	−171.95 (18)	C10—C9—C14—C13	−2.3 (4)
C15—N4—N5—C17	1.2 (2)	C8—C9—C14—C13	−179.6 (2)
C15—N4—N5—C27	173.9 (2)	N5—N4—C15—C16	−0.8 (2)
C5—N1—C1—C2	0.3 (3)	N5—N4—C15—C1	179.42 (19)
C5—N1—C1—C15	−178.48 (18)	N1—C1—C15—N4	−176.9 (2)
N1—C1—C2—C3	0.0 (3)	C2—C1—C15—N4	4.3 (3)
C15—C1—C2—C3	178.8 (2)	N1—C1—C15—C16	3.4 (3)
C1—C2—C3—C4	0.3 (3)	C2—C1—C15—C16	−175.4 (2)
C2—C3—C4—C5	−1.1 (3)	N4—C15—C16—C17	0.2 (3)
C1—N1—C5—C4	−1.1 (3)	C1—C15—C16—C17	179.9 (2)

C1—N1—C5—C6	179.08 (18)	N4—N5—C17—C16	−1.1 (3)
C3—C4—C5—N1	1.5 (3)	C27—N5—C17—C16	−173.0 (2)
C3—C4—C5—C6	−178.7 (2)	N4—N5—C17—C18	179.9 (2)
N3—N2—C6—C7	0.9 (2)	C27—N5—C17—C18	8.0 (4)
N3—N2—C6—C5	179.74 (19)	C15—C16—C17—N5	0.5 (2)
N1—C5—C6—N2	−164.57 (19)	C15—C16—C17—C18	179.4 (2)
C4—C5—C6—N2	15.6 (3)	N5—C17—C18—C19	−107.9 (3)
N1—C5—C6—C7	14.0 (3)	C16—C17—C18—C19	73.4 (3)
C4—C5—C6—C7	−165.8 (2)	N5—C17—C18—C23	73.3 (3)
N2—C6—C7—C8	−0.9 (3)	C16—C17—C18—C23	−105.4 (3)
C5—C6—C7—C8	−179.6 (2)	C23—C18—C19—C20	−1.4 (4)
N2—N3—C8—C7	0.0 (2)	C17—C18—C19—C20	179.8 (2)
C24—N3—C8—C7	170.1 (2)	C18—C19—C20—C21	0.8 (4)
N2—N3—C8—C9	178.7 (2)	C19—C20—C21—C22	−0.1 (4)
C24—N3—C8—C9	−11.2 (4)	C20—C21—C22—C23	0.1 (4)
C6—C7—C8—N3	0.5 (2)	C21—C22—C23—C18	−0.7 (4)
C6—C7—C8—C9	−178.1 (2)	C19—C18—C23—C22	1.4 (3)
N3—C8—C9—C10	135.3 (2)	C17—C18—C23—C22	−179.8 (2)
C7—C8—C9—C10	−46.4 (4)	N2—N3—C24—C25	57.3 (3)
N3—C8—C9—C14	−47.5 (3)	C8—N3—C24—C25	−112.3 (3)
C7—C8—C9—C14	130.9 (3)	N2—N3—C24—C26	−68.7 (3)
C14—C9—C10—C11	1.4 (4)	C8—N3—C24—C26	121.7 (2)
C8—C9—C10—C11	178.8 (2)	N4—N5—C27—C28	52.8 (3)
C9—C10—C11—C12	0.3 (5)	C17—N5—C27—C28	−135.8 (3)
C10—C11—C12—C13	−1.2 (5)	N4—N5—C27—C29	−71.5 (3)
C11—C12—C13—C14	0.3 (5)	C17—N5—C27—C29	99.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···*Cg*1^{i}	0.93	2.86	3.710 (3)	153

Symmetry code: (i) −*x*+1, −*y*, −*z*.