Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,4-Bis(2-pyridyl)-5-(3-pyridyl)-4*H*-1,2,4-triazole

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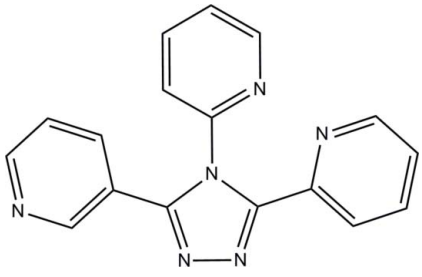
Received 13 April 2011; accepted 15 April 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.050; wR factor = 0.129; data-to-parameter ratio = 11.9.

In the title molecule, $C_{17}H_{12}N_6$, the 2-pyridyl rings in the 3- and 4-positions and the 3-pyridyl ring in the 5-position make dihedral angles of 29.78 (16), 67.06 (16) and 32.97 (16)°, respectively, with the triazole group. The dihedral angle between the two 2-pyridyl rings is 65.72 (15)°. The dihedral angles between the 3-pyridyl ring and the two 2-pyridyl rings in the 3- and 4-positions are 61.28 (15) and 63.11 (15)°, respectively. In the crystal, C—H$\cdots\pi$ and π–π interactions [centroid-centroid distance = 3.6248 (19) Å] link the molecules, forming a two-dimensional network.

Related literature

For the synthesis of the title compound, see: Klingele & Brooker (2004). For related structures and background references, see: Guo *et al.* (2010); Yang *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{12}N_6$
M_r = 300.33
Monoclinic, $P2_1/c$
a = 5.7621 (9) Å
b = 15.250 (3) Å
c = 16.640 (3) Å
β = 105.023 (5)°
V = 1412.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.982
6865 measured reflections
2496 independent reflections
1407 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.129
S = 1.08
2496 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

*Cg*2 and *Cg*4 are the centroids of the N1/C8–C12 and N6/C13–C17 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots Cg2^{i}$	0.93	2.94	3.765 (4)	149
C4—H4$\cdots Cg4$	0.93	2.92	3.616 (3)	133

Symmetry code: (i) $x-1, -y+\frac{1}{2}, z-\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was supported financially by Tianjin Normal University (52X09004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2269).

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supporting information

Acta Cryst. (2011). E**67**, o1189 [doi:10.1107/S1600536811014140]

3,4-Bis(2-pyridyl)-5-(3-pyridyl)-4*H*-1,2,4-triazole

Jing-Min Wu, Wei Guo and Cheng-Peng Li

S1. Comment

In continuation of our work on tripyridine-substituted triazole derivatives (Guo *et al.*, 2010; Yang *et al.*, 2010), we now describe the synthesis and crystal structure of the title compound. It consists of two 2-pyridyl groups and one 3-pyridyl ring attached to a triazole ring (Fig. 1).

The three pyridyl rings in the 3-, 4-, and 5-positions deviate from the triazole ring by 29.78 (16)°, 67.06 (16)°, and 32.97 (16)°, respectively. The dihedral angle between the two 2-pyridyl groups is 65.72 (15)°. In addition, the dihedral angles between the 3-pyridyl ring and the two 2-pyridyl rings in the 3- and 4-positions are 61.28 (15)° and 63.11 (15)°, respectively.

In the crystal, there exists a π–π interaction involving the 2-pyridyl rings in 3-positions of molecules related by an inversion center [centroid-centroid distance = 3.6248 (19) Å]. The molecular packing is also stabilized by two types of C—H···π interactions; the intramolecular C4—H4···*Cg*4 [*Cg*4 is the centroid of pyridine ring (N6/C13-C17)] and the intermolecular C3—H3···*Cg*2^{i} [*Cg*2 is the centroid of pyridine ring (N1/C8-C12)] interactions (see Table 1 and Fig. 2 for details). This leads to the formation of a two-dimensional network.

S2. Experimental

The title compound was prepared from a mixture of *N*-(pyridin-2-yl)pyridine-2-carbothioamide and pyridine-3-carbohydrazide using the method described by Klingele *et al.* (2004).

S3. Refinement

All H atoms were initially located in a difference Fourier map. The C—H atoms were then constrained to ideal geometry and refined as riding atoms: C—H = 0.93 Å, with U_{iso}(H) = 1.2*U*eq(C).

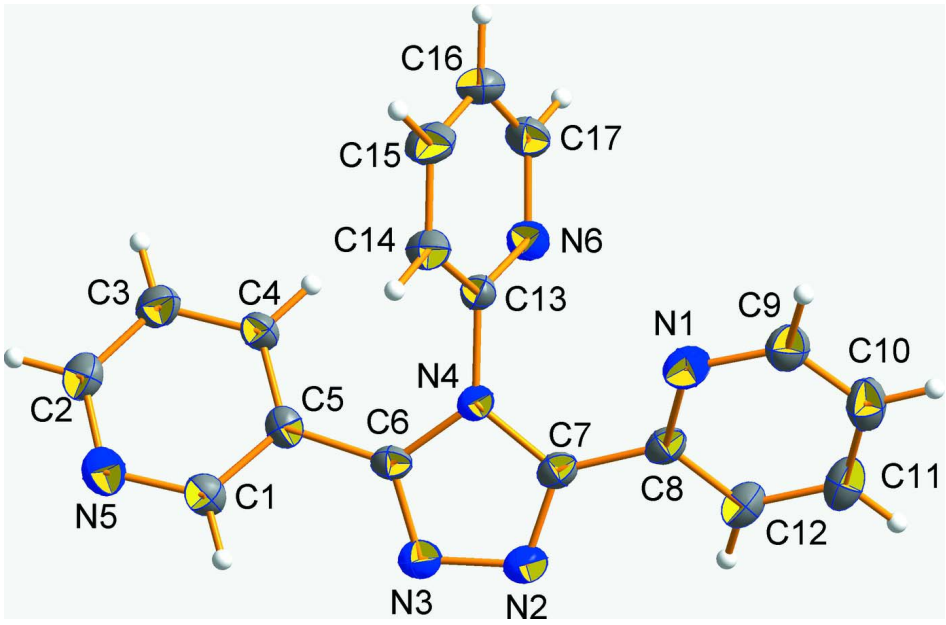

Figure 1

Molecular structure of the title molecule showing the numbering scheme and displacement ellipsoids drawn at the 30% probability level.

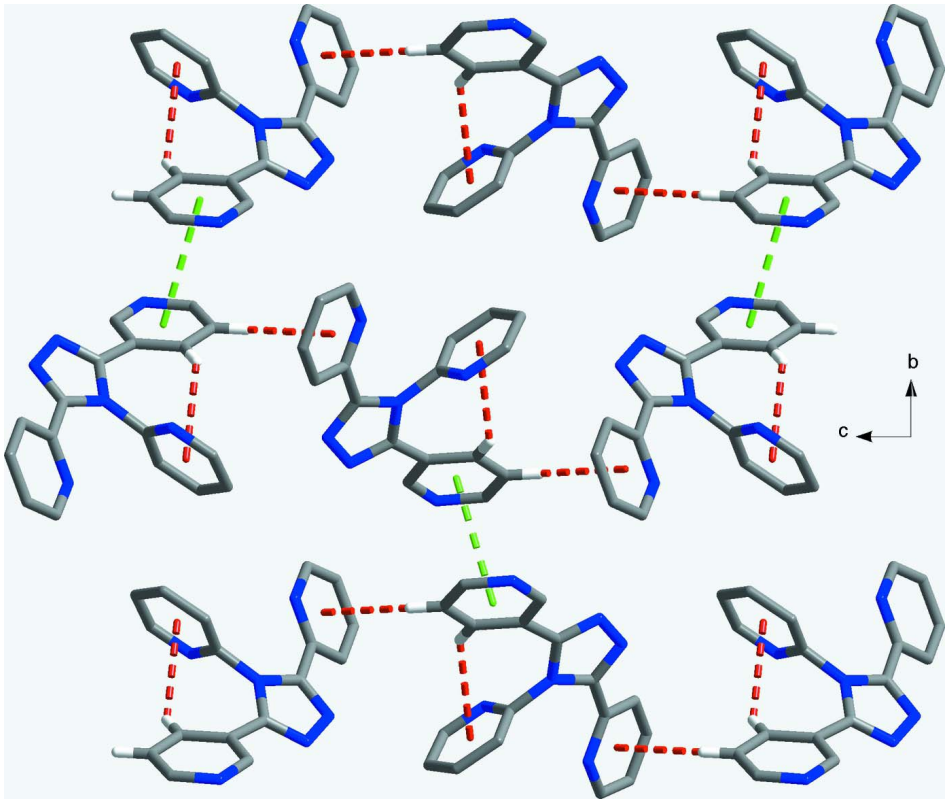

Figure 2

A view along the *a* axis of the C—H···π (red dashed lines) and π–π (green dashed lines) interactions in the crystal packing of the title compound (see Table 1 for details).

3,4-Bis(2-pyridyl)-5-(3-pyridyl)-4*H*-1,2,4-triazole

Crystal data

$C_{17}H_{12}N_6$
$M_r = 300.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.7621$ (9) Å
$b = 15.250$ (3) Å
$c = 16.640$ (3) Å
$\beta = 105.023$ (5)°
$V = 1412.2$ (4) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.413$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1374 reflections
$\theta = 2.5$–$22.0°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Block, colourless
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.975$, $T_{max} = 0.982$
6865 measured reflections
2496 independent reflections
1407 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -5 \rightarrow 6$
$k = -18 \rightarrow 18$
$l = -19 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.129$
$S = 1.08$
2496 reflections
209 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
$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 0.6358P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0124 (17)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.8676 (5)	0.8964 (2)	0.69324 (16)	0.0620 (8)
N2	0.6880 (5)	0.68510 (18)	0.75149 (15)	0.0531 (7)
N3	0.4816 (5)	0.63917 (17)	0.71292 (16)	0.0525 (7)

N4	0.5220 (4)	0.74876 (16)	0.63138 (13)	0.0402 (6)
N5	−0.2135 (5)	0.57144 (18)	0.56487 (19)	0.0646 (8)
N6	0.6492 (4)	0.79687 (17)	0.51665 (15)	0.0527 (7)
C1	−0.0072 (6)	0.6053 (2)	0.6135 (2)	0.0524 (8)
H1	0.0195	0.6012	0.6710	0.063*
C2	−0.2431 (6)	0.5784 (2)	0.4816 (2)	0.0572 (9)
H2	−0.3822	0.5557	0.4463	0.069*
C3	−0.0776 (6)	0.6174 (2)	0.4471 (2)	0.0585 (9)
H3	−0.1055	0.6206	0.3896	0.070*
C4	0.1285 (5)	0.6514 (2)	0.49739 (19)	0.0479 (8)
H4	0.2420	0.6781	0.4746	0.057*
C5	0.1657 (5)	0.64570 (19)	0.58214 (19)	0.0436 (8)
C6	0.3855 (5)	0.6773 (2)	0.64142 (17)	0.0418 (7)
C7	0.7095 (5)	0.7501 (2)	0.70183 (18)	0.0438 (8)
C8	0.9078 (5)	0.8133 (2)	0.72220 (17)	0.0449 (8)
C9	1.0537 (7)	0.9537 (2)	0.7146 (2)	0.0653 (10)
H9	1.0303	1.0110	0.6951	0.078*
C10	1.2745 (6)	0.9304 (3)	0.7638 (2)	0.0680 (10)
H10	1.3979	0.9715	0.7771	0.082*
C11	1.3130 (6)	0.8464 (3)	0.7933 (2)	0.0639 (10)
H11	1.4620	0.8297	0.8268	0.077*
C12	1.1283 (5)	0.7875 (2)	0.77272 (19)	0.0547 (9)
H12	1.1503	0.7303	0.7925	0.066*
C13	0.4854 (5)	0.80537 (19)	0.55974 (17)	0.0395 (7)
C14	0.2895 (6)	0.8593 (2)	0.5398 (2)	0.0525 (9)
H14	0.1811	0.8621	0.5726	0.063*
C15	0.2599 (7)	0.9094 (2)	0.4689 (2)	0.0685 (11)
H15	0.1300	0.9475	0.4529	0.082*
C16	0.4233 (7)	0.9027 (2)	0.4218 (2)	0.0689 (11)
H16	0.4053	0.9358	0.3737	0.083*
C17	0.6135 (6)	0.8462 (2)	0.4475 (2)	0.0625 (10)
H17	0.7234	0.8417	0.4154	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0686 (19)	0.064 (2)	0.0505 (18)	0.0029 (17)	0.0101 (14)	−0.0032 (15)
N2	0.0565 (17)	0.0589 (18)	0.0425 (15)	0.0064 (15)	0.0106 (13)	0.0061 (14)
N3	0.0548 (17)	0.0546 (18)	0.0482 (17)	0.0043 (14)	0.0133 (14)	0.0059 (14)
N4	0.0393 (14)	0.0462 (15)	0.0344 (14)	0.0038 (12)	0.0082 (11)	0.0007 (12)
N5	0.0652 (19)	0.0567 (19)	0.072 (2)	−0.0041 (15)	0.0186 (17)	−0.0024 (16)
N6	0.0512 (16)	0.0626 (19)	0.0468 (16)	0.0017 (13)	0.0174 (13)	0.0008 (14)
C1	0.059 (2)	0.049 (2)	0.053 (2)	−0.0062 (17)	0.0216 (18)	−0.0058 (16)
C2	0.049 (2)	0.058 (2)	0.060 (2)	0.0030 (17)	0.0076 (18)	−0.0059 (18)
C3	0.054 (2)	0.073 (3)	0.049 (2)	0.0043 (18)	0.0135 (18)	0.0028 (17)
C4	0.0454 (19)	0.054 (2)	0.0474 (19)	−0.0025 (16)	0.0183 (16)	0.0041 (15)
C5	0.0412 (18)	0.0410 (19)	0.0516 (19)	0.0034 (15)	0.0175 (16)	−0.0033 (15)
C6	0.0460 (18)	0.0450 (19)	0.0377 (17)	0.0049 (16)	0.0166 (14)	0.0034 (15)

C7	0.0448 (18)	0.0488 (19)	0.0374 (17)	0.0069 (16)	0.0103 (14)	−0.0016 (16)
C8	0.0463 (18)	0.051 (2)	0.0362 (17)	0.0074 (16)	0.0092 (14)	−0.0033 (15)
C9	0.074 (3)	0.060 (2)	0.057 (2)	−0.011 (2)	0.008 (2)	−0.0068 (18)
C10	0.061 (2)	0.079 (3)	0.064 (2)	−0.018 (2)	0.016 (2)	−0.024 (2)
C11	0.050 (2)	0.074 (3)	0.062 (2)	0.003 (2)	0.0043 (18)	−0.019 (2)
C12	0.052 (2)	0.058 (2)	0.050 (2)	0.0095 (18)	0.0043 (16)	−0.0075 (16)
C13	0.0370 (16)	0.0458 (19)	0.0362 (16)	−0.0002 (15)	0.0105 (14)	−0.0012 (14)
C14	0.0479 (19)	0.059 (2)	0.053 (2)	0.0133 (17)	0.0176 (16)	0.0079 (17)
C15	0.065 (2)	0.068 (3)	0.067 (2)	0.019 (2)	0.008 (2)	0.020 (2)
C16	0.072 (3)	0.081 (3)	0.050 (2)	−0.005 (2)	0.010 (2)	0.022 (2)
C17	0.065 (2)	0.081 (3)	0.047 (2)	−0.014 (2)	0.0237 (18)	0.0002 (19)

Geometric parameters (Å, º)

N1—C8	1.354 (4)	C4—H4	0.9300
N1—C9	1.357 (4)	C5—C6	1.470 (4)
N2—C7	1.316 (4)	C7—C8	1.467 (4)
N2—N3	1.386 (3)	C8—C12	1.386 (4)
N3—C6	1.311 (3)	C9—C10	1.369 (5)
N4—C7	1.373 (3)	C9—H9	0.9300
N4—C6	1.379 (4)	C10—C11	1.371 (5)
N4—C13	1.442 (3)	C10—H10	0.9300
N5—C2	1.355 (4)	C11—C12	1.366 (4)
N5—C1	1.355 (4)	C11—H11	0.9300
N6—C13	1.331 (3)	C12—H12	0.9300
N6—C17	1.345 (4)	C13—C14	1.367 (4)
C1—C5	1.384 (4)	C14—C15	1.378 (4)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.370 (4)	C15—C16	1.376 (5)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.366 (4)	C16—C17	1.373 (5)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.373 (4)	C17—H17	0.9300
C8—N1—C9	117.3 (3)	N1—C8—C7	118.8 (3)
C7—N2—N3	107.4 (2)	C12—C8—C7	119.3 (3)
C6—N3—N2	107.8 (2)	N1—C9—C10	122.6 (3)
C7—N4—C6	104.8 (2)	N1—C9—H9	118.7
C7—N4—C13	127.7 (2)	C10—C9—H9	118.7
C6—N4—C13	127.4 (2)	C9—C10—C11	119.7 (3)
C2—N5—C1	116.1 (3)	C9—C10—H10	120.2
C13—N6—C17	115.7 (3)	C11—C10—H10	120.2
N5—C1—C5	123.3 (3)	C12—C11—C10	118.8 (3)
N5—C1—H1	118.3	C12—C11—H11	120.6
C5—C1—H1	118.3	C10—C11—H11	120.6
N5—C2—C3	123.1 (3)	C11—C12—C8	119.8 (3)
N5—C2—H2	118.5	C11—C12—H12	120.1
C3—C2—H2	118.5	C8—C12—H12	120.1

C4—C3—C2	119.8 (3)	N6—C13—C14	125.8 (3)
C4—C3—H3	120.1	N6—C13—N4	114.5 (2)
C2—C3—H3	120.1	C14—C13—N4	119.7 (3)
C3—C4—C5	118.9 (3)	C13—C14—C15	116.9 (3)
C3—C4—H4	120.5	C13—C14—H14	121.6
C5—C4—H4	120.5	C15—C14—H14	121.6
C4—C5—C1	118.7 (3)	C16—C15—C14	119.7 (3)
C4—C5—C6	123.1 (3)	C16—C15—H15	120.1
C1—C5—C6	118.2 (3)	C14—C15—H15	120.1
N3—C6—N4	109.9 (3)	C17—C16—C15	118.6 (3)
N3—C6—C5	123.5 (3)	C17—C16—H16	120.7
N4—C6—C5	126.6 (3)	C15—C16—H16	120.7
N2—C7—N4	110.1 (3)	N6—C17—C16	123.4 (3)
N2—C7—C8	123.0 (3)	N6—C17—H17	118.3
N4—C7—C8	126.9 (3)	C16—C17—H17	118.3
N1—C8—C12	121.8 (3)		

C7—N2—N3—C6	0.2 (3)	C9—N1—C8—C12	1.0 (4)
C2—N5—C1—C5	0.5 (5)	C9—N1—C8—C7	178.7 (3)
C1—N5—C2—C3	−0.3 (5)	N2—C7—C8—N1	−149.0 (3)
N5—C2—C3—C4	0.0 (5)	N4—C7—C8—N1	30.4 (4)
C2—C3—C4—C5	0.1 (5)	N2—C7—C8—C12	28.8 (4)
C3—C4—C5—C1	0.2 (4)	N4—C7—C8—C12	−151.7 (3)
C3—C4—C5—C6	177.6 (3)	C8—N1—C9—C10	−0.4 (5)
N5—C1—C5—C4	−0.5 (5)	N1—C9—C10—C11	−0.1 (5)
N5—C1—C5—C6	−178.0 (3)	C9—C10—C11—C12	0.0 (5)
N2—N3—C6—N4	−0.7 (3)	C10—C11—C12—C8	0.5 (5)
N2—N3—C6—C5	178.8 (3)	N1—C8—C12—C11	−1.1 (5)
C7—N4—C6—N3	0.8 (3)	C7—C8—C12—C11	−178.8 (3)
C13—N4—C6—N3	176.5 (3)	C17—N6—C13—C14	−0.3 (4)
C7—N4—C6—C5	−178.6 (3)	C17—N6—C13—N4	177.2 (3)
C13—N4—C6—C5	−3.0 (4)	C7—N4—C13—N6	65.1 (4)
C4—C5—C6—N3	−145.5 (3)	C6—N4—C13—N6	−109.6 (3)
C1—C5—C6—N3	31.9 (4)	C7—N4—C13—C14	−117.1 (3)
C4—C5—C6—N4	33.9 (5)	C6—N4—C13—C14	68.2 (4)
C1—C5—C6—N4	−148.7 (3)	N6—C13—C14—C15	−0.2 (5)
N3—N2—C7—N4	0.3 (3)	N4—C13—C14—C15	−177.6 (3)
N3—N2—C7—C8	179.8 (3)	C13—C14—C15—C16	0.5 (5)
C6—N4—C7—N2	−0.7 (3)	C14—C15—C16—C17	−0.4 (5)
C13—N4—C7—N2	−176.3 (3)	C13—N6—C17—C16	0.5 (5)
C6—N4—C7—C8	179.8 (3)	C15—C16—C17—N6	−0.2 (5)
C13—N4—C7—C8	4.2 (5)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg4 are the centroids of the N1/C8–C12 and N6/C13–C17 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*2^{i}	0.93	2.94	3.765 (4)	149

C4—H4···*Cg*4	0.93	2.92	3.616 (3)	133

Symmetry code: (i) $x-1, -y+1/2, z-3/2$.