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4-(1*H*-Indol-3-yl)-2,6-bis(pyrazin-2-yl)pyridine

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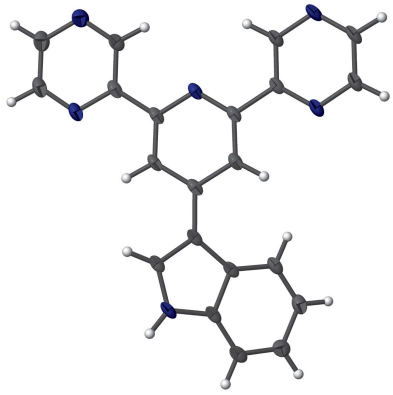
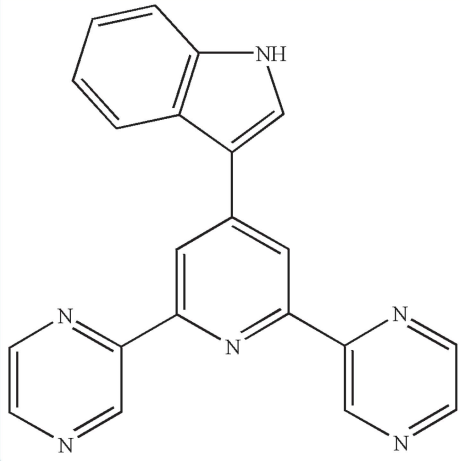
In the title compound, $C_{21}H_{14}N_6$, the pyridine ring and two pyrazine rings are nearly coplanar [dihedral angles = 2.03 (7) and 1.60 (7)°], while the dihedral angle between the indole ring system and the pyridine ring is 29.04 (6)°. In the crystal, molecules are linked by N—H···N hydrogen bonds, which generate [$\bar{1}$10] chains. The packing is consolidated by C—H···N hydrogen bonds and aromatic π–π stacking, generating a three-dimensional network.

3D view



Chemical scheme



Structure description

Pyridine/pyrazine ligands have attracted attention for the synthesis of transition-metal complexes with a variety of geometries (Sengupta *et al.* 2017; Rajput & Mukherjee 2013). Specifically, many terpyridine compounds, as convergent tridentate chelating N-donor ligands, have been synthesized and their coordination chemistries have been explored (Yin *et al.* 2015; Constable 2007; Wild *et al.* 2011). However, there is less research about the dipyrazinylpyridine compounds, which are close analogues of the terpyridines (Dai *et al.* 2010; Li *et al.* 2017).

The molecular structure of the title compound is illustrated in Fig. 1. The pyridine ring and the N1 and N4 pyrazine rings are nearly coplanar [dihedral angles = 2.03 (7) and 1.60 (7)°, respectively], indicating significant electronic conjugation, but the indole ring system deviates significantly from the pyridine ring [dihedral angle = 29.04 (6)°].

The N1 and N4 atoms of the pyrazine rings adopt *trans* conformations to the N3 atom of the central pyridine moiety, which does not seem to be a good conformation for a tridentate ligand. However, the single bond between the pyrazine ring and pyridine ring is easy to rotate freely in solution, so some tridentate metal complexes can also be obtained under appropriate conditions, for example the reported cadmium complexes with dipyrazinylpyridine ligands (Xie *et al.* 2016; Dai *et al.* 2010).

In the crystal, the N4 and N5 atoms in one pyrazine moiety accept C3—H3···N4 and N6—H6*A*···N5 hydrogen bonds, as shown in Fig. 2 and Table 1. The N—H···N hydrogen

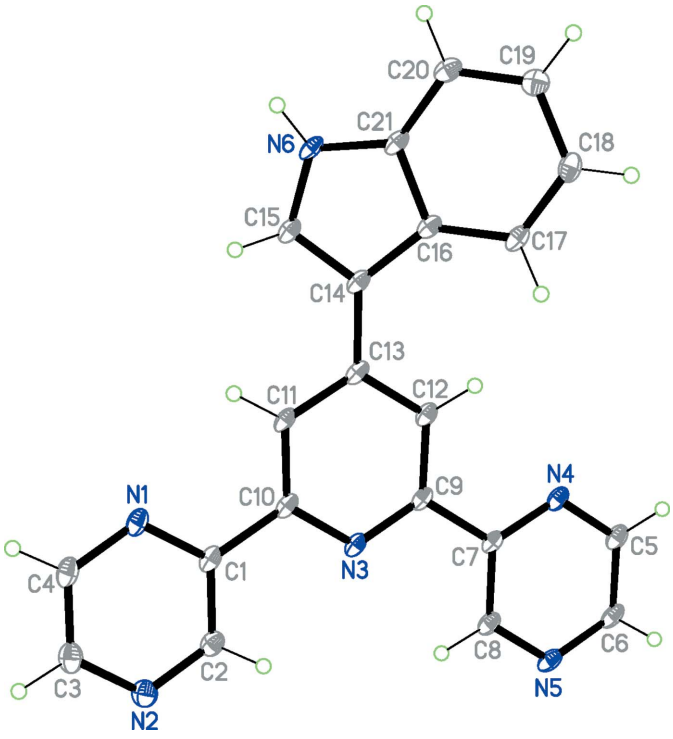


Figure 1
View of the title compound, shown with 50% probability displacement ellipsoids.

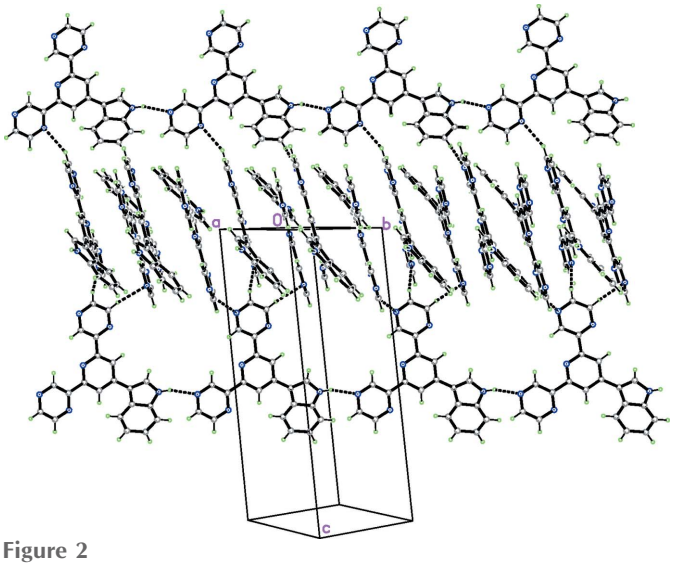


Figure 2
The hydrogen-bonding interactions (dashed lines) in the title compound.

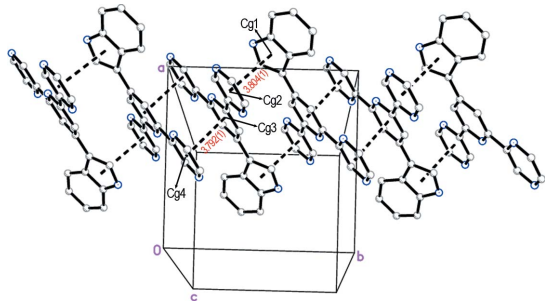


Figure 3
The aromatic π–π interactions (dashed lines) in the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6A···N5^{i}	0.88	2.18	3.0190 (19)	160
C3—H3···N4^{ii}	0.95	2.54	3.425 (2)	155

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{14}N_6$
M_r	350.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	8.5560 (17), 8.9820 (18), 22.130 (4)
β (°)	98.28 (3)
V (Å^3)	1683.0 (6)
Z	4
Radiation type	Synchrotron, λ = 0.710 Å
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Mar555
Absorption correction	Multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.983, 0.987
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5341, 2943, 2746
R_{int}	0.136
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.161, 1.04
No. of reflections	2943
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.23

Computer programs: mar555, *HKL-2000* (Minor *et al.*, 2000), *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

bonds generate [1$\bar{1}$0] chains, which are cross-linked by the C—H···N bonds. Moreover, π–π stacking interactions between the pyrazine and pyridine rings are also observed (Fig. 3). The ring-centroid distances between the pyrazine ring and the

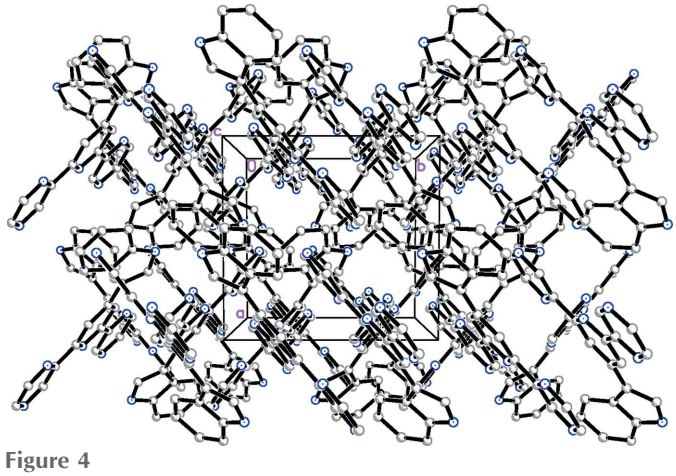


Figure 4
The packing of the title compound.

adjacent pyridine and indole rings are 3.7925 (11) and 3.8044 (11) Å, respectively. The overall packing is shown in Fig. 4.

Synthesis and crystallization

0.1 mmol of $Pt(DMSO)_2Cl_2$ (DMSO = dimethyl sulfoxide) was added to a stirring solution of 2,6-bis(2-pyrazinyl)-4-(indol-1-yl)pyridine (0.1 mmol) in 15 ml of methanol. The solution was refluxed at 338 K for 5 h under a nitrogen atmosphere, cooled slowly and filtered. The filtrate was kept at room temperature and after about two weeks colorless block-shaped crystals of the title compound were collected by filtration.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One outlier with was removed from the final refinement. DISP instructions appropriate to the synchrotron wavelength were used in the refinement.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180492 [https://doi.org/10.1107/S2414314618004923]

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Crystal data

$C_{21}H_{14}N_6$
M_r = 350.38
Monoclinic, $P2_1/c$
a = 8.5560 (17) Å
b = 8.9820 (18) Å
c = 22.130 (4) Å
β = 98.28 (3)°
V = 1683.0 (6) Å^3
Z = 4
$F(000)$ = 728
D_x = 1.383 Mg m^{-3}
Synchrotron radiation, λ = 0.710 Å
Cell parameters from 8169 reflections
θ = 2.4–29.5°
μ = 0.09 mm^{-1}
T = 100 K
Block, colorless
0.20 × 0.20 × 0.15 mm

Data collection

Mar555 diffractometer
Radiation source: synchrotron, 3W1A at BSRF
oscillation mode scans
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)
T_{min} = 0.983, T_{max} = 0.987
5341 measured reflections
2943 independent reflections
2746 reflections with $I > 2\sigma(I)$
R_{int} = 0.136
θ_{max} = 25.1°, θ_{min} = 2.5°
h = 0→10
k = −10→10
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.161
S = 1.04
2943 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 0.3936P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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	1.03422 (15)	0.27853 (16)	0.37871 (6)	0.0206 (3)
C2	1.15461 (16)	0.20143 (18)	0.35555 (6)	0.0238 (4)
H2	1.2202	0.1367	0.3820	0.029*
C3	1.08481 (17)	0.3086 (2)	0.26267 (7)	0.0300 (4)
H3	1.0992	0.3226	0.2213	0.036*
C4	0.96495 (18)	0.38505 (19)	0.28541 (7)	0.0291 (4)
H4	0.8996	0.4499	0.2589	0.035*
C5	1.29758 (16)	−0.05260 (17)	0.66620 (7)	0.0246 (4)
H5	1.2917	−0.0663	0.7084	0.029*
C6	1.41440 (16)	−0.12564 (17)	0.64057 (7)	0.0243 (4)
H6	1.4869	−0.1872	0.6658	0.029*
C7	1.20761 (15)	0.05372 (16)	0.57419 (6)	0.0187 (3)
C8	1.32527 (15)	−0.02103 (17)	0.54830 (6)	0.0225 (4)
H8	1.3323	−0.0068	0.5062	0.027*
C9	1.09203 (15)	0.15450 (16)	0.53679 (6)	0.0184 (3)
C10	1.00918 (15)	0.26218 (16)	0.44353 (6)	0.0192 (3)
C11	0.89131 (15)	0.34194 (16)	0.46693 (6)	0.0195 (3)
H11	0.8246	0.4075	0.4413	0.023*
C12	0.97715 (15)	0.22973 (16)	0.56388 (6)	0.0202 (3)
H12	0.9706	0.2164	0.6060	0.024*
C13	0.87170 (15)	0.32504 (16)	0.52825 (6)	0.0193 (3)
C14	0.74714 (15)	0.40481 (16)	0.55418 (6)	0.0195 (3)
C15	0.68268 (14)	0.53939 (16)	0.53282 (6)	0.0194 (3)
H15	0.7116	0.5926	0.4990	0.023*
C16	0.66742 (14)	0.36347 (17)	0.60505 (6)	0.0191 (3)
C17	0.67148 (16)	0.23950 (17)	0.64456 (6)	0.0234 (4)
H17	0.7442	0.1608	0.6416	0.028*
C18	0.56950 (17)	0.23335 (18)	0.68735 (7)	0.0264 (4)
H18	0.5737	0.1505	0.7142	0.032*
C19	0.45876 (16)	0.34818 (19)	0.69195 (6)	0.0265 (4)
H19	0.3885	0.3407	0.7214	0.032*
C20	0.45158 (16)	0.47124 (18)	0.65405 (6)	0.0244 (4)
H20	0.3771	0.5484	0.6569	0.029*
C21	0.55699 (15)	0.47885 (16)	0.61143 (6)	0.0203 (3)
N1	0.93776 (14)	0.37132 (15)	0.34299 (6)	0.0252 (3)
N2	1.18128 (14)	0.21474 (17)	0.29804 (6)	0.0288 (4)
N3	1.10821 (12)	0.16745 (14)	0.47763 (5)	0.0191 (3)
N4	1.19234 (13)	0.03709 (14)	0.63322 (5)	0.0218 (3)
N5	1.42847 (14)	−0.11231 (15)	0.58137 (6)	0.0251 (3)
N6	0.57157 (13)	0.58462 (14)	0.56739 (5)	0.0211 (3)
H6A	0.5176	0.6682	0.5624	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0160 (6)	0.0159 (7)	0.0264 (7)	−0.0035 (6)	−0.0083 (5)	0.0009 (6)
C2	0.0202 (7)	0.0233 (8)	0.0256 (7)	0.0010 (6)	−0.0049 (5)	−0.0004 (6)
C3	0.0279 (7)	0.0348 (10)	0.0245 (7)	−0.0040 (7)	−0.0059 (6)	0.0019 (7)
C4	0.0278 (7)	0.0289 (9)	0.0275 (7)	0.0004 (7)	−0.0068 (6)	0.0066 (7)
C5	0.0237 (7)	0.0203 (8)	0.0264 (7)	0.0027 (6)	−0.0077 (5)	0.0028 (6)
C6	0.0213 (7)	0.0170 (8)	0.0309 (7)	0.0048 (6)	−0.0092 (5)	0.0007 (6)
C7	0.0166 (6)	0.0125 (7)	0.0243 (7)	−0.0010 (6)	−0.0056 (5)	−0.0011 (6)
C8	0.0196 (7)	0.0189 (8)	0.0265 (7)	0.0039 (6)	−0.0055 (5)	0.0006 (6)
C9	0.0160 (6)	0.0119 (7)	0.0246 (7)	−0.0011 (6)	−0.0058 (5)	−0.0003 (6)
C10	0.0152 (6)	0.0135 (7)	0.0259 (7)	−0.0015 (5)	−0.0077 (5)	−0.0003 (6)
C11	0.0151 (6)	0.0141 (7)	0.0262 (7)	0.0005 (6)	−0.0071 (5)	0.0015 (6)
C12	0.0183 (6)	0.0160 (7)	0.0238 (7)	−0.0003 (6)	−0.0058 (5)	0.0007 (6)
C13	0.0145 (6)	0.0130 (7)	0.0276 (7)	−0.0011 (6)	−0.0068 (5)	−0.0014 (6)
C14	0.0157 (6)	0.0160 (8)	0.0236 (7)	0.0011 (6)	−0.0086 (5)	−0.0024 (6)
C15	0.0152 (6)	0.0160 (7)	0.0238 (7)	−0.0006 (5)	−0.0084 (5)	−0.0011 (6)
C16	0.0147 (6)	0.0163 (7)	0.0233 (7)	0.0008 (5)	−0.0077 (5)	−0.0037 (6)
C17	0.0214 (7)	0.0174 (8)	0.0287 (7)	0.0025 (6)	−0.0055 (5)	0.0010 (6)
C18	0.0264 (7)	0.0223 (8)	0.0280 (7)	−0.0031 (6)	−0.0048 (6)	0.0041 (6)
C19	0.0195 (7)	0.0320 (9)	0.0263 (7)	−0.0019 (6)	−0.0025 (5)	−0.0027 (7)
C20	0.0176 (7)	0.0252 (8)	0.0273 (7)	0.0031 (6)	−0.0073 (5)	−0.0044 (7)
C21	0.0158 (6)	0.0173 (7)	0.0239 (7)	0.0014 (6)	−0.0099 (5)	−0.0028 (6)
N1	0.0234 (6)	0.0234 (7)	0.0262 (6)	0.0021 (5)	−0.0054 (4)	0.0045 (6)
N2	0.0246 (6)	0.0338 (8)	0.0262 (6)	0.0005 (6)	−0.0025 (5)	−0.0012 (6)
N3	0.0157 (5)	0.0137 (6)	0.0253 (6)	−0.0007 (5)	−0.0057 (4)	0.0007 (5)
N4	0.0192 (6)	0.0176 (7)	0.0258 (6)	0.0023 (5)	−0.0066 (4)	0.0017 (5)
N5	0.0207 (6)	0.0203 (7)	0.0312 (7)	0.0073 (5)	−0.0064 (5)	−0.0005 (6)
N6	0.0173 (6)	0.0154 (6)	0.0273 (6)	0.0038 (5)	−0.0080 (4)	−0.0008 (5)

Geometric parameters (Å, º)

C1—N1	1.3463 (18)	C10—C11	1.396 (2)
C1—C2	1.398 (2)	C11—C13	1.399 (2)
C1—C10	1.488 (2)	C11—H11	0.9500
C2—N2	1.330 (2)	C12—C13	1.4014 (19)
C2—H2	0.9500	C12—H12	0.9500
C3—N2	1.348 (2)	C13—C14	1.468 (2)
C3—C4	1.388 (2)	C14—C15	1.383 (2)
C3—H3	0.9500	C14—C16	1.446 (2)
C4—N1	1.334 (2)	C15—N6	1.3650 (19)
C4—H4	0.9500	C15—H15	0.9500
C5—N4	1.3429 (18)	C16—C17	1.413 (2)
C5—C6	1.384 (2)	C16—C21	1.423 (2)
C5—H5	0.9500	C17—C18	1.378 (2)
C6—N5	1.338 (2)	C17—H17	0.9500
C6—H6	0.9500	C18—C19	1.414 (2)

C7—N4	1.3399 (19)	C18—H18	0.9500
C7—C8	1.399 (2)	C19—C20	1.384 (2)
C7—C9	1.4989 (18)	C19—H19	0.9500
C8—N5	1.3422 (18)	C20—C21	1.397 (2)
C8—H8	0.9500	C20—H20	0.9500
C9—N3	1.3412 (19)	C21—N6	1.380 (2)
C9—C12	1.397 (2)	N6—H6A	0.8800
C10—N3	1.3518 (18)		

N1—C1—C2	120.87 (13)	C11—C13—C12	117.03 (13)
N1—C1—C10	117.77 (13)	C11—C13—C14	121.42 (12)
C2—C1—C10	121.36 (12)	C12—C13—C14	121.55 (13)
N2—C2—C1	122.89 (13)	C15—C14—C16	106.31 (12)
N2—C2—H2	118.6	C15—C14—C13	124.70 (13)
C1—C2—H2	118.6	C16—C14—C13	129.00 (13)
N2—C3—C4	121.44 (14)	N6—C15—C14	110.13 (13)
N2—C3—H3	119.3	N6—C15—H15	124.9
C4—C3—H3	119.3	C14—C15—H15	124.9
N1—C4—C3	122.71 (14)	C17—C16—C21	118.03 (13)
N1—C4—H4	118.6	C17—C16—C14	135.37 (14)
C3—C4—H4	118.6	C21—C16—C14	106.53 (12)
N4—C5—C6	121.94 (13)	C18—C17—C16	119.68 (15)
N4—C5—H5	119.0	C18—C17—H17	120.2
C6—C5—H5	119.0	C16—C17—H17	120.2
N5—C6—C5	122.08 (13)	C17—C18—C19	121.15 (15)
N5—C6—H6	119.0	C17—C18—H18	119.4
C5—C6—H6	119.0	C19—C18—H18	119.4
N4—C7—C8	121.51 (12)	C20—C19—C18	120.72 (14)
N4—C7—C9	117.16 (12)	C20—C19—H19	119.6
C8—C7—C9	121.33 (13)	C18—C19—H19	119.6
N5—C8—C7	121.69 (13)	C19—C20—C21	118.14 (14)
N5—C8—H8	119.2	C19—C20—H20	120.9
C7—C8—H8	119.2	C21—C20—H20	120.9
N3—C9—C12	123.70 (12)	N6—C21—C20	130.04 (14)
N3—C9—C7	116.02 (12)	N6—C21—C16	107.61 (12)
C12—C9—C7	120.28 (12)	C20—C21—C16	122.26 (14)
N3—C10—C11	122.97 (13)	C4—N1—C1	116.21 (13)
N3—C10—C1	115.76 (12)	C2—N2—C3	115.88 (13)
C11—C10—C1	121.26 (12)	C9—N3—C10	117.06 (12)
C10—C11—C13	119.86 (12)	C7—N4—C5	116.42 (12)
C10—C11—H11	120.1	C6—N5—C8	116.34 (13)
C13—C11—H11	120.1	C15—N6—C21	109.40 (12)
C9—C12—C13	119.33 (13)	C15—N6—H6A	125.3
C9—C12—H12	120.3	C21—N6—H6A	125.3
C13—C12—H12	120.3		

N1—C1—C2—N2	0.2 (2)	C15—C14—C16—C21	−0.06 (14)
C10—C1—C2—N2	−179.25 (13)	C13—C14—C16—C21	−179.99 (12)

N2—C3—C4—N1	0.1 (2)	C21—C16—C17—C18	0.3 (2)
N4—C5—C6—N5	−0.6 (2)	C14—C16—C17—C18	−176.23 (15)
N4—C7—C8—N5	−0.2 (2)	C16—C17—C18—C19	0.9 (2)
C9—C7—C8—N5	−179.50 (12)	C17—C18—C19—C20	−1.0 (2)
N4—C7—C9—N3	−178.98 (12)	C18—C19—C20—C21	−0.2 (2)
C8—C7—C9—N3	0.3 (2)	C19—C20—C21—N6	177.50 (13)
N4—C7—C9—C12	1.70 (19)	C19—C20—C21—C16	1.5 (2)
C8—C7—C9—C12	−179.00 (13)	C17—C16—C21—N6	−178.34 (11)
N1—C1—C10—N3	179.73 (12)	C14—C16—C21—N6	−0.88 (14)
C2—C1—C10—N3	−0.8 (2)	C17—C16—C21—C20	−1.56 (19)
N1—C1—C10—C11	−1.0 (2)	C14—C16—C21—C20	175.90 (12)
C2—C1—C10—C11	178.47 (13)	C3—C4—N1—C1	0.3 (2)
N3—C10—C11—C13	−0.2 (2)	C2—C1—N1—C4	−0.4 (2)
C1—C10—C11—C13	−179.44 (12)	C10—C1—N1—C4	179.03 (13)
N3—C9—C12—C13	−0.2 (2)	C1—C2—N2—C3	0.2 (2)
C7—C9—C12—C13	179.10 (12)	C4—C3—N2—C2	−0.4 (2)
C10—C11—C13—C12	1.8 (2)	C12—C9—N3—C10	1.8 (2)
C10—C11—C13—C14	−178.80 (12)	C7—C9—N3—C10	−177.52 (11)
C9—C12—C13—C11	−1.6 (2)	C11—C10—N3—C9	−1.6 (2)
C9—C12—C13—C14	178.97 (12)	C1—C10—N3—C9	177.70 (11)
C11—C13—C14—C15	−27.0 (2)	C8—C7—N4—C5	1.2 (2)
C12—C13—C14—C15	152.40 (13)	C9—C7—N4—C5	−179.48 (12)
C11—C13—C14—C16	152.92 (14)	C6—C5—N4—C7	−0.8 (2)
C12—C13—C14—C16	−27.7 (2)	C5—C6—N5—C8	1.6 (2)
C16—C14—C15—N6	1.00 (14)	C7—C8—N5—C6	−1.2 (2)
C13—C14—C15—N6	−179.07 (12)	C14—C15—N6—C21	−1.60 (15)
C15—C14—C16—C17	176.75 (14)	C20—C21—N6—C15	−174.92 (13)
C13—C14—C16—C17	−3.2 (3)	C16—C21—N6—C15	1.52 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···N5^{i}	0.88	2.18	3.0190 (19)	160
C3—H3···N4^{ii}	0.95	2.54	3.425 (2)	155

Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) *x*, −*y*+1/2, *z*−1/2.