data reports

Crystal structure of 5-(4,5-dihydro-1*H*-imidazol-2-yl)-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyrazin-6-amine

Joel T. Mague,[a] Shaaban K. Mohamed,[b,c] Mehmet Akkurt,[d] Talaat I. El-Emary[e] and Mustafa R. Albayati[f]*

[a]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA, [b]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [c]Chemistry Department, Faculty of Science, Minia University, 61519 El-Minia, Egypt, [d]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [e]Department of Chemistry, Faculty of Science, Assiut University, 71515 Assiut, Egypt, and [f]Kirkuk University, College of Science, Department of Chemistry, Kirkuk, Iraq. *Correspondence e-mail: shaabankamel@yahoo.com
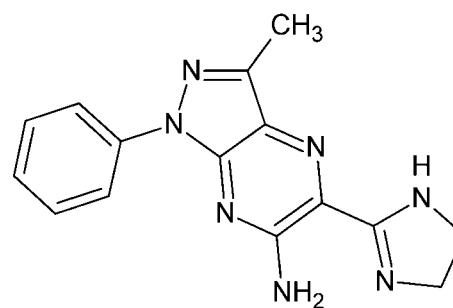
In the title compound, $C_{15}H_{15}N_7$, the phenyl ring is inclined by 19.86 (5)° to the mean plane of the pyrazolo[3,4-*b*]pyrazine core. In the crystal, N—H···N and C—H···N hydrogen bonds form [010] chains, which stack *via* π–π interactions [centroid–centroid distance between the pyrazole rings = 3.4322 (7) Å].

1. Related literature

For the synthesis of similar pyrazolo[3,4-*b*]pyrazines, see: El-Emary & El-Kashef (2013). For different biological and industrial applications of pyrazolopyrazine scaffold compounds, see: El-Emary *et al.* (1998); El-Kashef *et al.* (2000); El-Emary (2006); Rangnekar (1990).

2. Experimental

2.1. Crystal data

$C_{15}H_{15}N_7$	$V = 2754.00\ (10)$ Å³
$M_r = 293.34$	$Z = 8$
Monoclinic, $C2/c$	Cu $K\alpha$ radiation
$a = 7.9412\ (2)$ Å	$\mu = 0.75$ mm⁻¹
$b = 15.7078\ (3)$ Å	$T = 150$ K
$c = 22.3276\ (4)$ Å	$0.15 \times 0.10 \times 0.05$ mm
$\beta = 98.573\ (1)°$	

2.2. Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer	21033 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)	2685 independent reflections
$T_{min} = 0.93$, $T_{max} = 0.97$	2335 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.031$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	201 parameters
$wR(F^2) = 0.094$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{max} = 0.23$ e Å⁻³
2685 reflections	$\Delta\rho_{min} = -0.17$ e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N5[i]	0.95	2.56	3.3483 (17)	140
N5—H5B···N2[ii]	0.91	2.31	3.1702 (15)	158
N5—H5A···N6	0.91	1.97	2.7111 (15)	138

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT*; program(s) used to solve structure: *SHELXT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL2014* (Sheldrick, 2008).

Acknowledgements

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supporting information

Crystal structure of 5-(4,5-dihydro-1*H*-imidazol-2-yl)-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyrazin-6-amine

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S1. Comment

Pyrazine scaffold compounds are an interesting class of fused heterocyclic compounds due to their diverse properties in medicinal and applied chemistry. Pyrazolo[3,4-*b*]pyrazine derivatives have been reported to act as blood platelet aggregation inhibitors and bone metabolism improvers (El-Emary & El-Kashef, 2013). They also show antifungal and antiparasitic activities (El-Emary *et al.*, 1998; El-Kashef *et al.*, 2000; El-Emary, 2006). In addition, they are used as dye dispersants and as fluorescents (Rangnekar, 1990). In view of this medicinal importance, the crystal structure determination of the title compound was carried out and the results are presented here.
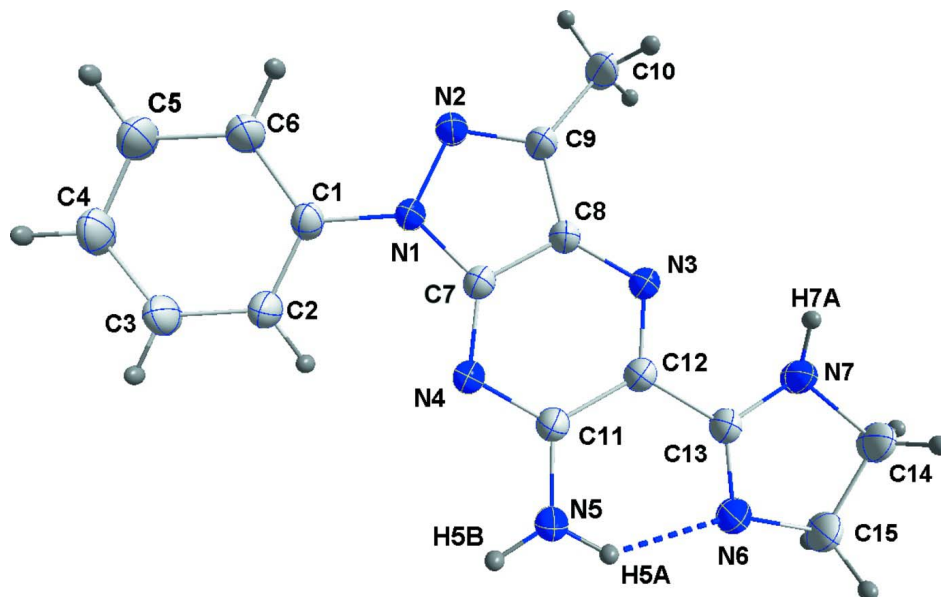
In the title compound, the pyrazolo[3,4-*b*]pyrazine core is planar (r.m.s. deviation 0.0089) with the phenyl ring inclined by 19.86 (5)° to it. An intramolecular N5—H5a···N6 hydrogen bond (Table 1 and Fig. 1) keeps the dihydroimidazolyl substituent nearly coplanar with the core. Intermolecular N5—H5b···N2 and C6—H6···N5 hydrogen bonds form chains of molecules (Table 1 and Fig. 2) which stack *via* π–π interactions between pyrazine rings (Cg^i···Cg^{ii} = Cg^{iii}··· Cg^{iv} = 3.43 Å. Cg^i: 0.5 - *x*, 1/2 + *y*, 0.5 - *z*; Cg^{ii}: -1/2 + *x*, 1/2 + *y*, *z*; Cg^{iii}: 0.5 - *x*, -1/2 + *y*, 0.5 - *z*; Cg^{iv}: -1/2 + *x*, -1/2 + *y*, *z*. Figs. 3 and 4). The chains run approximately parallel to (102).

S2. Experimental

The title compound has been prepared according to our reported method (El-Kashef *et al.*, 2000). The product was crystallized from dioxan to furnish a good yield (68%) of colourles crystals (m.p. 503–505 K) which were of suffiecient quality for X-ray diffraction.

S3. Refinement

H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

Figure 1

The title molecule with numbering scheme and 50% probability ellipsoids. The intramolecular hydrogen bond is shown as a blue dotted line.

Figure 2

Plan view of the chain showing N—H⋯N and C—H⋯N hydrogen bonds as blue and black dotted lines, respectively.

Figure 3

Elevation view of two chains showing the π-π interactions as green dotted lines.

Figure 4

Packing viewed down the *a* axis.

5-(4,5-Dihydro-1*H*-imidazol-2-yl)-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyrazin-6-amine

Crystal data

C₁₅H₁₅N₇

$C_{15}H_{15}N_7$
$M_r = 293.34$
Monoclinic, *C*2/*c*
$a = 7.9412$ (2) Å
$b = 15.7078$ (3) Å
$c = 22.3276$ (4) Å

$\beta = 98.573$ (1)°
$V = 2754.00$ (10) Å^3
$Z = 8$
$F(000) = 1232$
$D_x = 1.415$ Mg m^{-3}
Cu *Kα* radiation, $\lambda = 1.54178$ Å

Cell parameters from 9946 reflections

$\theta = 4.0–71.7°$

$\mu = 0.75$ mm^{-1}

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS
diffractometer

Radiation source: INCOATEC IµS micro–focus
source

Mirror monochromator

Detector resolution: 10.4167 pixels mm^{-1}

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2014)

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.094$

$S = 1.04$

2685 reflections

201 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

$T = 150$ K

Block, colourless

$0.15 \times 0.10 \times 0.05$ mm

$T_{min} = 0.93$, $T_{max} = 0.97$

21033 measured reflections

2685 independent reflections

2335 reflections with $I > 2\sigma(I)$

$R_{int} = 0.031$

$\theta_{max} = 72.0°$, $\theta_{min} = 4.0°$

$h = -9 \rightarrow 9$

$k = -19 \rightarrow 18$

$l = -25 \rightarrow 27$

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 1.7272P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.23$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: *SHELXL2014* (Sheldrick,
2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$

Extinction coefficient: 0.00012 (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 $F^2 > \sigma(F^2)$ 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 base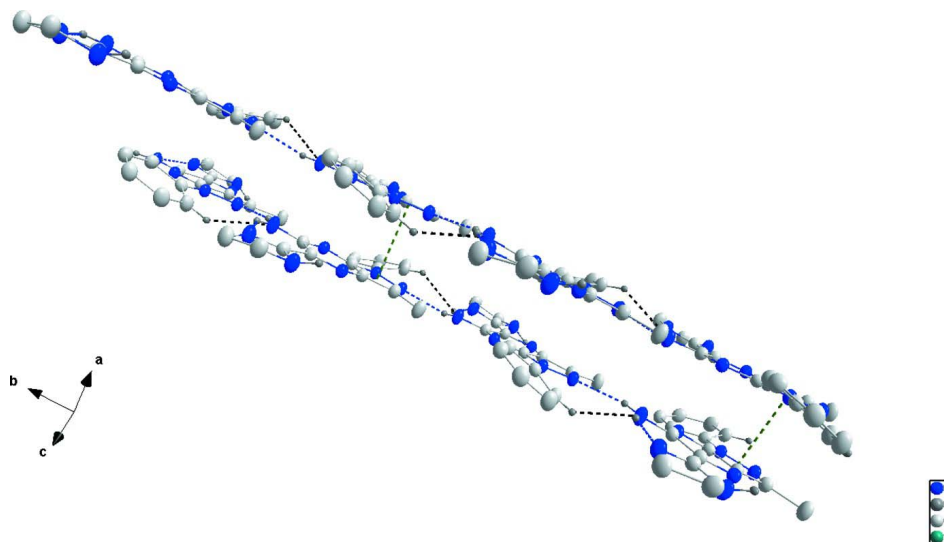d on ALL data will be even larger. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.98 Å) while those attached to nitrogen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.
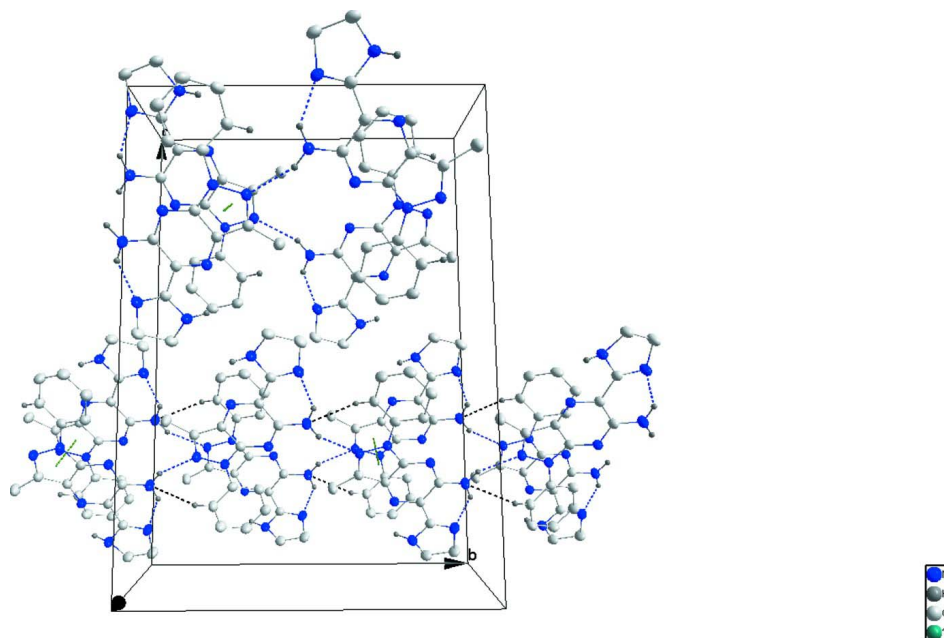
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.21440 (13)	0.23938 (6)	0.22995 (4)	0.0252 (2)
N2	0.24278 (14)	0.15429 (6)	0.24683 (5)	0.0284 (3)
N3	0.49830 (13)	0.27132 (6)	0.36366 (5)	0.0255 (2)
N4	0.31514 (13)	0.37679 (6)	0.27055 (4)	0.0258 (2)
N5	0.43603 (15)	0.49390 (7)	0.32160 (5)	0.0350 (3)
H5A	0.5051	0.5149	0.3545	0.042*
H5B	0.3806	0.5295	0.2931	0.042*
N6	0.62895 (15)	0.47203 (7)	0.43134 (5)	0.0345 (3)

N7	0.69317 (15)	0.33776 (7)	0.46313 (5)	0.0339 (3)
H7A	0.7265	0.2859	0.4511	0.041*
C1	0.10360 (15)	0.25899 (8)	0.17597 (5)	0.0255 (3)
C2	0.03232 (16)	0.33968 (8)	0.16704 (6)	0.0292 (3)
H2	0.0600	0.3829	0.1967	0.035*
C3	−0.07919 (17)	0.35656 (9)	0.11468 (6)	0.0325 (3)
H3	−0.1269	0.4119	0.1083	0.039*
C4	−0.12216 (18)	0.29404 (9)	0.07151 (6)	0.0366 (3)
H4	−0.2016	0.3057	0.0363	0.044*
C5	−0.04798 (19)	0.21408 (9)	0.08019 (6)	0.0382 (3)
H5	−0.0757	0.1711	0.0504	0.046*
C6	0.06600 (18)	0.19648 (8)	0.13184 (6)	0.0322 (3)
H6	0.1183	0.1421	0.1371	0.039*
C7	0.30685 (15)	0.29182 (8)	0.27108 (5)	0.0241 (3)
C8	0.39641 (15)	0.23910 (8)	0.31557 (5)	0.0251 (3)
C9	0.35066 (16)	0.15415 (8)	0.29763 (6)	0.0278 (3)
C10	0.4086 (2)	0.07325 (9)	0.32887 (7)	0.0377 (3)
H10A	0.3465	0.0253	0.3079	0.057*
H10B	0.3866	0.0753	0.3709	0.057*
H10C	0.5309	0.0659	0.3284	0.057*
C11	0.41803 (16)	0.40912 (8)	0.31815 (5)	0.0260 (3)
C12	0.50810 (15)	0.35545 (8)	0.36559 (5)	0.0253 (3)
C13	0.61270 (16)	0.39176 (8)	0.41964 (5)	0.0263 (3)
C14	0.80754 (19)	0.38977 (9)	0.50567 (6)	0.0366 (3)
H14A	0.9268	0.3854	0.4980	0.044*
H14B	0.8018	0.3736	0.5482	0.044*
C15	0.73523 (19)	0.47864 (9)	0.49128 (6)	0.0380 (3)
H15A	0.6658	0.4970	0.5223	0.046*
H15B	0.8283	0.5203	0.4901	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0278 (5)	0.0214 (5)	0.0242 (5)	−0.0011 (4)	−0.0036 (4)	−0.0001 (4)
N2	0.0326 (6)	0.0213 (5)	0.0288 (6)	−0.0016 (4)	−0.0037 (4)	0.0005 (4)
N3	0.0263 (5)	0.0237 (5)	0.0250 (5)	−0.0011 (4)	−0.0008 (4)	−0.0008 (4)
N4	0.0269 (6)	0.0230 (5)	0.0256 (5)	−0.0006 (4)	−0.0019 (4)	−0.0005 (4)
N5	0.0429 (7)	0.0222 (5)	0.0345 (6)	0.0006 (5)	−0.0123 (5)	−0.0005 (4)
N6	0.0385 (6)	0.0279 (6)	0.0329 (6)	−0.0012 (5)	−0.0082 (5)	−0.0059 (5)
N7	0.0434 (7)	0.0270 (6)	0.0269 (6)	−0.0027 (5)	−0.0087 (5)	−0.0004 (4)
C1	0.0244 (6)	0.0276 (6)	0.0233 (6)	−0.0040 (5)	−0.0007 (5)	0.0017 (5)
C2	0.0300 (7)	0.0289 (7)	0.0269 (6)	0.0004 (5)	−0.0014 (5)	−0.0016 (5)
C3	0.0319 (7)	0.0319 (7)	0.0315 (7)	0.0023 (5)	−0.0024 (6)	0.0031 (5)
C4	0.0370 (7)	0.0396 (8)	0.0289 (7)	−0.0038 (6)	−0.0095 (6)	0.0032 (6)
C5	0.0465 (8)	0.0337 (7)	0.0301 (7)	−0.0065 (6)	−0.0088 (6)	−0.0033 (6)
C6	0.0387 (7)	0.0251 (6)	0.0300 (7)	−0.0030 (5)	−0.0035 (6)	−0.0002 (5)
C7	0.0232 (6)	0.0249 (6)	0.0233 (6)	−0.0013 (5)	0.0009 (5)	−0.0011 (5)
C8	0.0260 (6)	0.0233 (6)	0.0245 (6)	0.0000 (5)	−0.0010 (5)	0.0002 (5)

C9	0.0300 (7)	0.0246 (6)	0.0270 (6)	−0.0013 (5)	−0.0018 (5)	−0.0002 (5)
C10	0.0463 (8)	0.0254 (7)	0.0364 (7)	−0.0021 (6)	−0.0108 (6)	0.0029 (5)
C11	0.0261 (6)	0.0244 (6)	0.0262 (6)	0.0006 (5)	−0.0004 (5)	−0.0016 (5)
C12	0.0251 (6)	0.0243 (6)	0.0253 (6)	−0.0011 (5)	0.0005 (5)	−0.0016 (5)
C13	0.0259 (6)	0.0268 (6)	0.0252 (6)	−0.0011 (5)	0.0007 (5)	−0.0008 (5)
C14	0.0408 (8)	0.0371 (7)	0.0280 (7)	−0.0054 (6)	−0.0075 (6)	−0.0028 (6)
C15	0.0398 (8)	0.0359 (7)	0.0339 (7)	−0.0033 (6)	−0.0089 (6)	−0.0089 (6)

Geometric parameters (Å, º)

N1—C7	1.3638 (15)	C3—C4	1.3826 (19)
N1—N2	1.3978 (14)	C3—H3	0.9500
N1—C1	1.4161 (16)	C4—C5	1.389 (2)
N2—C9	1.3158 (17)	C4—H4	0.9500
N3—C12	1.3241 (16)	C5—C6	1.3836 (19)
N3—C8	1.3435 (16)	C5—H5	0.9500
N4—C7	1.3365 (16)	C6—H6	0.9500
N4—C11	1.3401 (16)	C7—C8	1.4028 (17)
N5—C11	1.3404 (16)	C8—C9	1.4246 (17)
N5—H5A	0.9100	C9—C10	1.4891 (18)
N5—H5B	0.9099	C10—H10A	0.9800
N6—C13	1.2902 (17)	C10—H10B	0.9800
N6—C15	1.4755 (17)	C10—H10C	0.9800
N7—C13	1.3732 (16)	C11—C12	1.4554 (17)
N7—C14	1.4620 (17)	C12—C13	1.4741 (16)
N7—H7A	0.9099	C14—C15	1.525 (2)
C1—C2	1.3904 (18)	C14—H14A	0.9900
C1—C6	1.3916 (18)	C14—H14B	0.9900
C2—C3	1.3829 (18)	C15—H15A	0.9900
C2—H2	0.9500	C15—H15B	0.9900
C7—N1—N2	110.30 (10)	N3—C8—C7	121.67 (11)
C7—N1—C1	130.20 (10)	N3—C8—C9	132.50 (11)
N2—N1—C1	119.48 (10)	C7—C8—C9	105.83 (11)
C9—N2—N1	106.98 (10)	N2—C9—C8	110.29 (11)
C12—N3—C8	115.30 (10)	N2—C9—C10	121.41 (11)
C7—N4—C11	113.36 (10)	C8—C9—C10	128.29 (11)
C11—N5—H5A	116.9	C9—C10—H10A	109.5
C11—N5—H5B	122.3	C9—C10—H10B	109.5
H5A—N5—H5B	120.8	H10A—C10—H10B	109.5
C13—N6—C15	106.19 (11)	C9—C10—H10C	109.5
C13—N7—C14	107.03 (11)	H10A—C10—H10C	109.5
C13—N7—H7A	118.0	H10B—C10—H10C	109.5
C14—N7—H7A	120.9	N4—C11—N5	117.98 (11)
C2—C1—C6	120.12 (12)	N4—C11—C12	122.21 (11)
C2—C1—N1	120.56 (11)	N5—C11—C12	119.81 (11)
C6—C1—N1	119.31 (11)	N3—C12—C11	122.30 (11)
C3—C2—C1	119.46 (12)	N3—C12—C13	115.85 (11)

C3—C2—H2	120.3	C11—C12—C13	121.83 (11)
C1—C2—H2	120.3	N6—C13—N7	116.00 (11)
C4—C3—C2	120.89 (13)	N6—C13—C12	124.83 (11)
C4—C3—H3	119.6	N7—C13—C12	119.08 (11)
C2—C3—H3	119.6	N7—C14—C15	101.34 (10)
C3—C4—C5	119.33 (12)	N7—C14—H14A	111.5
C3—C4—H4	120.3	C15—C14—H14A	111.5
C5—C4—H4	120.3	N7—C14—H14B	111.5
C6—C5—C4	120.54 (13)	C15—C14—H14B	111.5
C6—C5—H5	119.7	H14A—C14—H14B	109.3
C4—C5—H5	119.7	N6—C15—C14	105.85 (10)
C5—C6—C1	119.60 (13)	N6—C15—H15A	110.6
C5—C6—H6	120.2	C14—C15—H15A	110.6
C1—C6—H6	120.2	N6—C15—H15B	110.6
N4—C7—N1	128.29 (11)	C14—C15—H15B	110.6
N4—C7—C8	125.12 (11)	H15A—C15—H15B	108.7
N1—C7—C8	106.59 (10)		
C7—N1—N2—C9	0.15 (14)	N1—N2—C9—C8	−0.06 (15)
C1—N1—N2—C9	179.34 (11)	N1—N2—C9—C10	179.61 (12)
C7—N1—C1—C2	−20.6 (2)	N3—C8—C9—N2	178.77 (13)
N2—N1—C1—C2	160.36 (11)	C7—C8—C9—N2	−0.05 (15)
C7—N1—C1—C6	159.58 (12)	N3—C8—C9—C10	−0.9 (2)
N2—N1—C1—C6	−19.42 (17)	C7—C8—C9—C10	−179.69 (14)
C6—C1—C2—C3	1.55 (19)	C7—N4—C11—N5	179.53 (11)
N1—C1—C2—C3	−178.23 (11)	C7—N4—C11—C12	−0.94 (17)
C1—C2—C3—C4	0.8 (2)	C8—N3—C12—C11	−1.44 (17)
C2—C3—C4—C5	−2.0 (2)	C8—N3—C12—C13	177.08 (10)
C3—C4—C5—C6	0.9 (2)	N4—C11—C12—N3	2.23 (19)
C4—C5—C6—C1	1.4 (2)	N5—C11—C12—N3	−178.24 (12)
C2—C1—C6—C5	−2.6 (2)	N4—C11—C12—C13	−176.20 (11)
N1—C1—C6—C5	177.17 (12)	N5—C11—C12—C13	3.32 (18)
C11—N4—C7—N1	179.70 (12)	C15—N6—C13—N7	0.00 (16)
C11—N4—C7—C8	−0.87 (18)	C15—N6—C13—C12	176.46 (12)
N2—N1—C7—N4	179.34 (12)	C14—N7—C13—N6	−12.26 (16)
C1—N1—C7—N4	0.3 (2)	C14—N7—C13—C12	171.07 (11)
N2—N1—C7—C8	−0.18 (13)	N3—C12—C13—N6	−175.55 (12)
C1—N1—C7—C8	−179.25 (12)	C11—C12—C13—N6	3.0 (2)
C12—N3—C8—C7	−0.33 (17)	N3—C12—C13—N7	0.80 (17)
C12—N3—C8—C9	−178.99 (13)	C11—C12—C13—N7	179.33 (11)
N4—C7—C8—N3	1.63 (19)	C13—N7—C14—C15	17.78 (15)
N1—C7—C8—N3	−178.84 (11)	C13—N6—C15—C14	11.67 (16)
N4—C7—C8—C9	−179.40 (12)	N7—C14—C15—N6	−17.76 (15)
N1—C7—C8—C9	0.14 (13)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N5[i]	0.95	2.56	3.3483 (17)	140
N5—H5B···N2[ii]	0.91	2.31	3.1702 (15)	158
N5—H5A···N6	0.91	1.97	2.7111 (15)	138

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