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N-(2-Phenylimidazo[1,2-*a*]pyridin-3-yl)-acetamide

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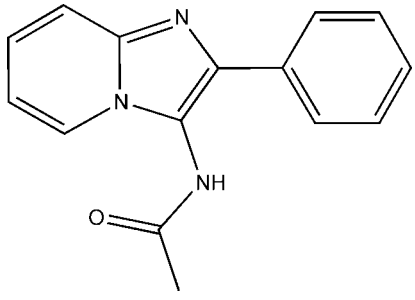
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.085; data-to-parameter ratio = 14.6.

The crystal structure of the title compound, $C_{15}H_{13}N_3O$, consists of columns of molecules that are interconnected by N—H···N hydrogen bonds in the direction of the b axis. The torsion angle between the imidazo[1,2-*a*]pyridine ring system and the phenyl ring is 9.04 (5)°.

Related literature

For general background, see Anaflous *et al.* (2004); Gueffier *et al.* (1998); Mavel *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{13}N_3O$
M_r = 251.3
Monoclinic, $P2_1/c$
a = 13.9680 (5) Å
b = 5.6784 (2) Å
c = 15.8145 (5) Å
β = 101.039 (3)°
V = 1231.13 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.58 × 0.25 × 0.17 mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer with Sapphire2 CCD detector
Absorption correction: none
15703 measured reflections
2556 independent reflections
1544 reflections with $I > 3\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 1.00
2556 reflections
175 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3n···N1^{i}	0.880 (12)	2.162 (12)	3.0219 (16)	165.4 (13)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg & Putz, 1999); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2112).

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supporting information

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N-(2-Phenylimidazo[1,2-*a*]pyridin-3-yl)acetamide

Abderrahmane Anaflous, Hanane Albay, Nour-eddine Benchat, Brahim El Bali, Michal Dušek and Karla Fejfarová

S1. Comment

In recent years, functionalized imidazo[1,2-*a*]pyridine and imidazo[1,2-*a*]pyrimidine systems attracted persistent interest due to their biological activities (Anaflous *et al.*, 2004 and reference herein). The screening of imidazo[1,2-*a*]pyridine derivatives against tuberculosis showed interesting results (Anaflous *et al.*, 2004) and many functionalized imidazo[1,2-*a*]pyridines bearing a thioether side chain at the 3 position are reported as highly active against human cytomegalovirus and /or varicella-zoster virus (Gueffier *et al.*, 1998 & Mavel *et al.*, 2002).

We report in the present paper on the synthesis and crystal structure of *N*-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetamide (I).

The molecules of the title compound are interconnected into columns extended along b by an N3—H3n···N1 hydrogen bonds (see Tab. 1). No bonding has been found between the columns that appear to be quite isolated.

Bonds and angles values are usual as those reported in similar compounds.

The torsion angle between the imidazo[1,2-*a*]pyridine and phenyl ring is 9.04 (5)°

S2. Experimental

The commercially available 2-phenylimidazo[1,2-*a*]pyridin-3-amine (0.50 g, 2.4 mmole) in toluene (10 ml, 94 mmole) was treated with acetic anhydride (0.3 ml, 3.2 mmole). The mixture was stirred for two hours. Toluene was eliminated under reduced pressure and the residue was washed with water to give, after drying, 0.45 g (1.8 mmole) of *N*-(2-phenyl-imidazo[1,2-*a*]pyridin-3-yl)acetamide as colorless crystals.

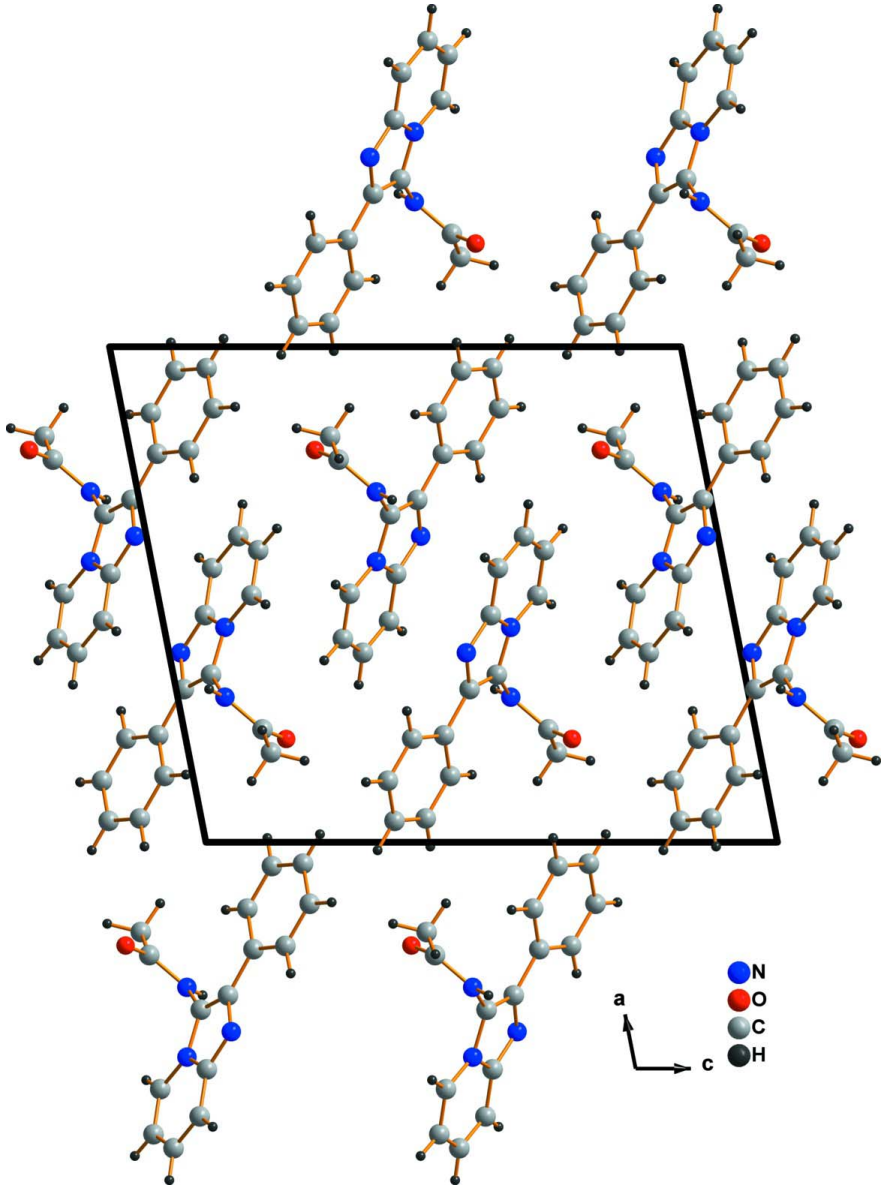

Figure 1

View of the unit cell of the title structure along the axis b

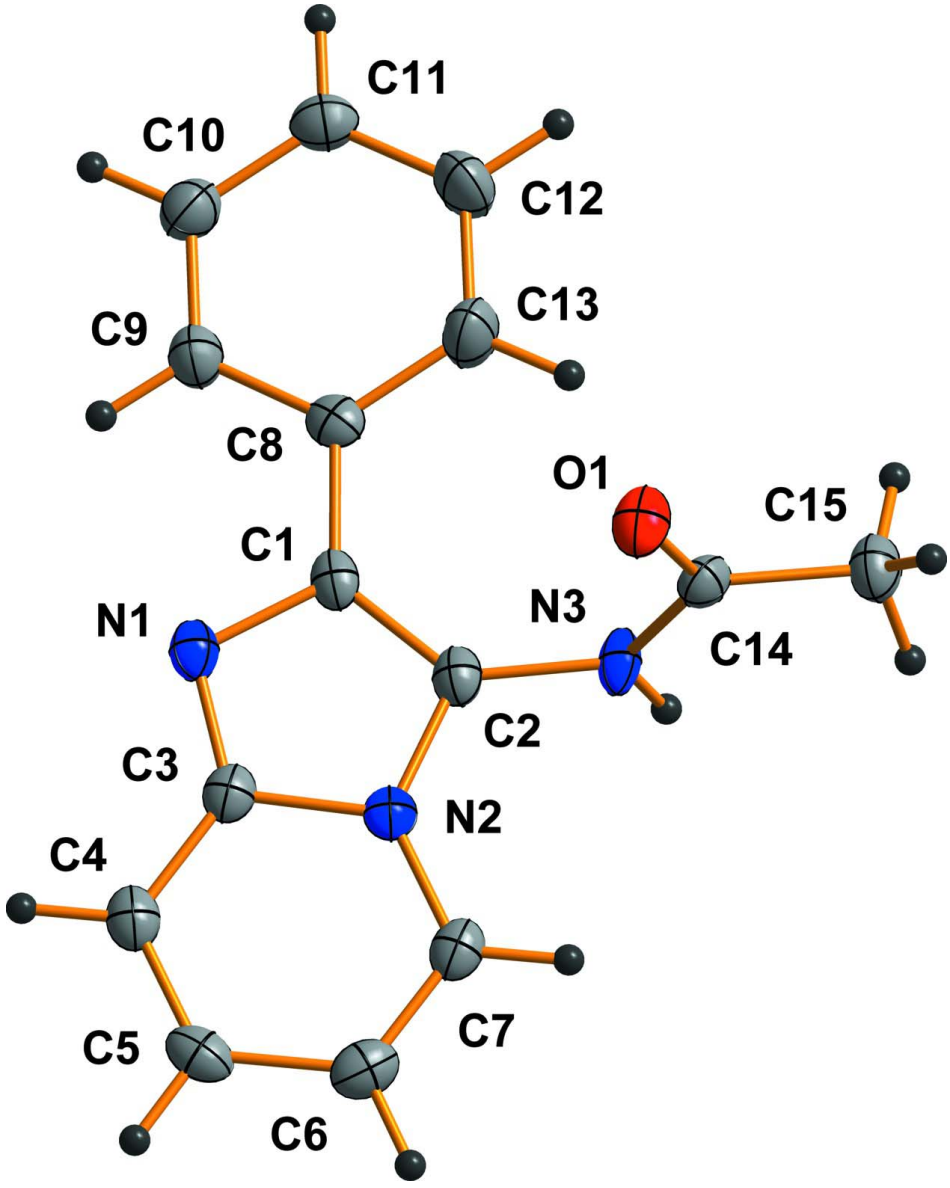

Figure 2

Asymetric unit of title compound, showing 50% displacement ellispoids for non-H atoms.

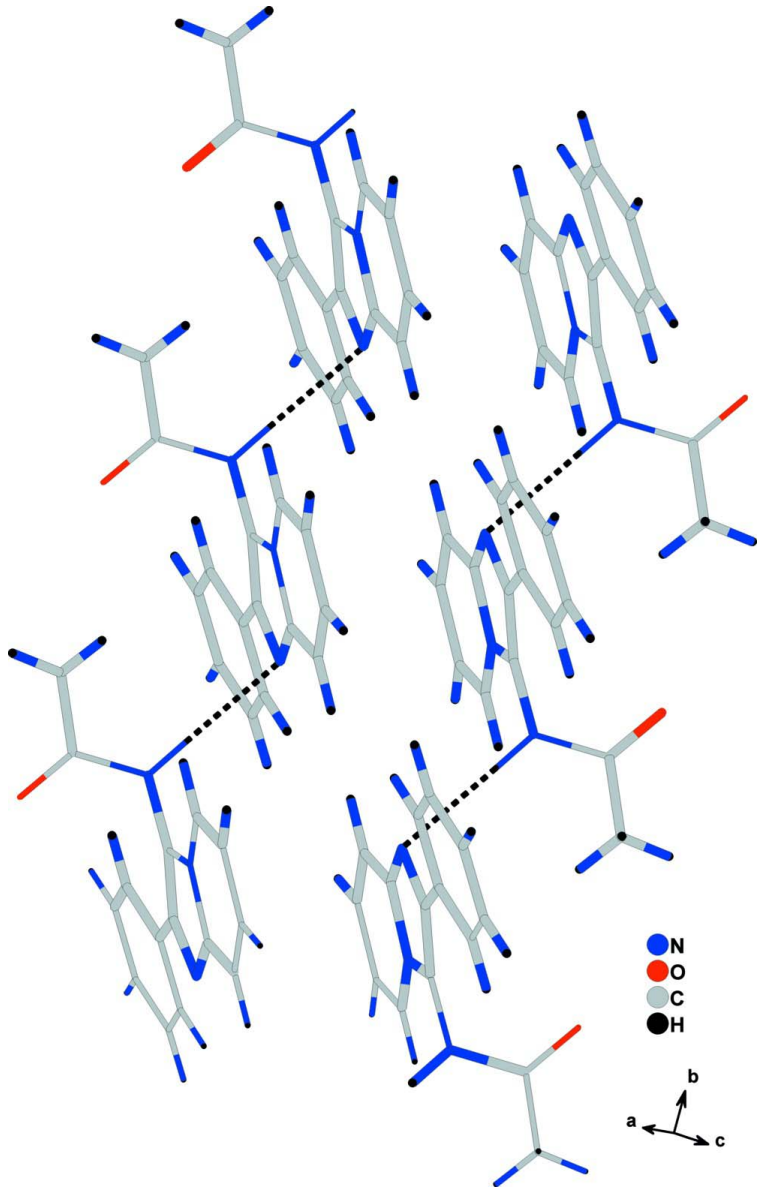

Figure 3

The columns of molecules showing N—H···N hydrogen bonds

N-(2-Phenylimidazo[1,2-*a*]pyridin-3-yl)acetamide

Crystal data

$C_{15}H_{13}N_3O$
$M_r = 251.3$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.9680\ (5)$ Å
$b = 5.6784\ (2)$ Å
$c = 15.8145\ (5)$ Å
$\beta = 101.039\ (3)°$
$V = 1231.13\ (7)$ Å^3
$Z = 4$

$F(000) = 528$
$D_x = 1.355$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4755 reflections
$\theta = 2.6–26.5°$
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Prism, colorless
0.58 × 0.25 × 0.17 mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer with Sapphire2 CCD detector
Radiation source: X-ray tube
Graphite monochromator
Detector resolution: 8.3438 pixels mm^{-1}
Rotation method data acquisition using ω scans
15703 measured reflections
2556 independent reflections
1544 reflections with $I > 3\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.6°$
$h = -17 \rightarrow 17$
$k = -7 \rightarrow 7$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.084$
$S = 1.00$
2556 reflections
175 parameters
1 restraint
45 constraints
H atoms treated by a mixture of independent and constrained refinement
Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(I) + 0.0016I^2]$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

Special details

Refinement. The refinement was carried out against all reflections. The conventional *R*-factor is always based on *F*. The goodness of fit as well as the weighted *R*-factor are based on *F* and F^2 for refinement carried out on *F* and F^2, respectively. The threshold expression is used only for calculating *R*-factors *etc*. and it is not relevant to the choice of reflections for refinement.
All the H atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. According to standard procedures for organic compounds the H atoms bonded to C atoms were constrained to ideal positions. The N—H distances were restrained to 0.87 Å with σ 0.01. The isotropic atomic displacement parameters of hydrogen atoms were evaluated as 1.2*U_{eq} of the parent atom.
The program used for refinement, Jana2006, uses the weighting scheme based on the experimental expectations, see _refine_ls_weighting_details, that does not force *S* to be one. Therefore the values of *S* are usually larger than the ones from the *SHELX* program.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.61764 (8)	−0.2561 (2)	0.47985 (7)	0.0230 (4)
N2	0.56626 (7)	0.05089 (18)	0.39364 (7)	0.0206 (4)
N3	0.70718 (11)	0.3084 (2)	0.41732 (9)	0.0235 (5)
O1	0.79160 (9)	0.1417 (2)	0.32433 (8)	0.0298 (4)
C1	0.69090 (11)	−0.0912 (2)	0.48648 (9)	0.0210 (5)
C2	0.66186 (9)	0.09842 (19)	0.43398 (8)	0.0224 (4)
C3	0.54173 (10)	−0.1658 (2)	0.42431 (9)	0.0211 (5)
C4	0.44673 (11)	−0.2519 (3)	0.39578 (9)	0.0238 (5)
C5	0.38234 (11)	−0.1217 (3)	0.33930 (9)	0.0262 (5)
C6	0.41070 (11)	0.0979 (2)	0.30893 (9)	0.0272 (5)
C7	0.50162 (10)	0.1807 (3)	0.33604 (9)	0.0233 (5)
C8	0.78417 (11)	−0.1346 (2)	0.54688 (10)	0.0220 (6)
C9	0.79074 (12)	−0.3221 (3)	0.60385 (10)	0.0285 (5)
C10	0.87592 (12)	−0.3699 (3)	0.66086 (10)	0.0317 (5)
C11	0.95689 (11)	−0.2316 (3)	0.66266 (10)	0.0290 (5)
C12	0.95210 (12)	−0.0434 (3)	0.60733 (10)	0.0373 (6)
C13	0.86634 (12)	0.0062 (3)	0.54974 (11)	0.0356 (6)

C14	0.77211 (11)	0.3171 (3)	0.36247 (10)	0.0220 (5)
C15	0.81873 (12)	0.5518 (3)	0.35553 (11)	0.0294 (6)
H3n	0.6911 (10)	0.4370 (19)	0.4423 (9)	0.0282*
H4	0.42756	−0.400812	0.415958	0.0285*
H5	0.317152	−0.17869	0.319756	0.0314*
H6	0.364663	0.187888	0.268776	0.0327*
H7	0.520896	0.328874	0.315284	0.028*
H9	0.734759	−0.420445	0.603502	0.0341*
H10	0.878784	−0.500882	0.699648	0.038*
H11	1.016393	−0.265961	0.702246	0.0348*
H12	1.008436	0.054304	0.608524	0.0447*
H13	0.863646	0.13862	0.511608	0.0427*
H15a	0.77381	0.67451	0.36305	0.0353*
H15b	0.876474	0.564915	0.399312	0.0353*
H15c	0.8358 (10)	0.5666 (19)	0.2998 (9)	0.0353*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0273 (7)	0.0188 (6)	0.0250 (7)	−0.0018 (5)	0.0100 (6)	−0.0017 (5)
N2	0.0230 (7)	0.0198 (6)	0.0205 (6)	0.0005 (5)	0.0079 (5)	−0.0023 (5)
N3	0.0343 (9)	0.0126 (7)	0.0271 (8)	−0.0014 (7)	0.0148 (7)	−0.0020 (7)
O1	0.0405 (7)	0.0228 (6)	0.0305 (7)	0.0012 (6)	0.0176 (6)	−0.0026 (5)
C1	0.0263 (9)	0.0171 (7)	0.0225 (8)	−0.0029 (7)	0.0119 (7)	−0.0042 (6)
C2	0.0267 (8)	0.0183 (6)	0.0245 (7)	−0.0015 (6)	0.0108 (6)	−0.0028 (5)
C3	0.0275 (9)	0.0186 (7)	0.0192 (8)	0.0014 (7)	0.0098 (7)	−0.0021 (6)
C4	0.0304 (9)	0.0210 (8)	0.0227 (8)	−0.0023 (7)	0.0120 (7)	−0.0040 (6)
C5	0.0217 (9)	0.0333 (8)	0.0247 (8)	−0.0023 (7)	0.0074 (7)	−0.0094 (7)
C6	0.0317 (8)	0.0309 (8)	0.0195 (8)	0.0080 (6)	0.0062 (7)	0.0003 (6)
C7	0.0319 (8)	0.0197 (8)	0.0207 (8)	0.0027 (7)	0.0112 (7)	−0.0005 (6)
C8	0.0226 (10)	0.0222 (8)	0.0222 (9)	0.0012 (7)	0.0068 (8)	−0.0058 (7)
C9	0.0296 (9)	0.0261 (9)	0.0308 (9)	−0.0033 (8)	0.0086 (7)	0.0015 (7)
C10	0.0338 (9)	0.0285 (8)	0.0327 (9)	0.0036 (7)	0.0061 (8)	0.0048 (7)
C11	0.0282 (8)	0.0324 (9)	0.0258 (8)	0.0039 (7)	0.0034 (7)	−0.0015 (7)
C12	0.0293 (10)	0.0377 (9)	0.0425 (10)	−0.0114 (8)	0.0013 (8)	0.0022 (7)
C13	0.0394 (10)	0.0306 (9)	0.0357 (10)	−0.0038 (8)	0.0040 (8)	0.0111 (8)
C14	0.0251 (10)	0.0210 (9)	0.0203 (8)	0.0030 (7)	0.0055 (7)	0.0034 (7)
C15	0.0335 (10)	0.0248 (10)	0.0331 (11)	−0.0032 (8)	0.0144 (9)	0.0020 (9)

Geometric parameters (Å, º)

N1—C1	1.3763 (18)	C6—H6	0.96
N1—C3	1.3424 (17)	C7—H7	0.96
N2—C2	1.3916 (15)	C8—C9	1.387 (2)
N2—C3	1.3894 (17)	C8—C13	1.393 (2)
N2—C7	1.3689 (16)	C9—C10	1.375 (2)
N3—C2	1.3984 (19)	C9—H9	0.96
N3—C14	1.371 (2)	C10—C11	1.373 (2)

N3—H3n	0.880 (12)	C10—H10	0.96
O1—C14	1.222 (2)	C11—C12	1.375 (2)
C1—C2	1.3727 (18)	C11—H11	0.96
C1—C8	1.481 (2)	C12—C13	1.388 (2)
C3—C4	1.405 (2)	C12—H12	0.96
C4—C5	1.359 (2)	C13—H13	0.96
C4—H4	0.96	C14—C15	1.497 (2)
C5—C6	1.419 (2)	C15—H15a	0.96
C5—H5	0.96	C15—H15b	0.96
C6—C7	1.345 (2)	C15—H15c	0.960 (15)

C1—N1—C3	105.82 (11)	C1—C8—C9	119.17 (14)
C2—N2—C3	106.91 (10)	C1—C8—C13	122.90 (14)
C2—N2—C7	130.80 (11)	C9—C8—C13	117.93 (14)
C3—N2—C7	122.27 (11)	C8—C9—C10	121.26 (15)
C2—N3—C14	121.89 (13)	C8—C9—H9	119.372
C2—N3—H3n	117.3 (9)	C10—C9—H9	119.371
C14—N3—H3n	120.8 (9)	C9—C10—C11	120.43 (14)
N1—C1—C2	110.99 (11)	C9—C10—H10	119.784
N1—C1—C8	119.03 (12)	C11—C10—H10	119.784
C2—C1—C8	129.96 (13)	C10—C11—C12	119.48 (13)
N2—C2—N3	120.55 (11)	C10—C11—H11	120.26
N2—C2—C1	105.77 (11)	C12—C11—H11	120.259
N3—C2—C1	133.68 (12)	C11—C12—C13	120.42 (15)
N1—C3—N2	110.49 (11)	C11—C12—H12	119.792
N1—C3—C4	131.02 (13)	C13—C12—H12	119.792
N2—C3—C4	118.48 (12)	C8—C13—C12	120.48 (15)
C3—C4—C5	119.18 (14)	C8—C13—H13	119.758
C3—C4—H4	120.41	C12—C13—H13	119.758
C5—C4—H4	120.41	N3—C14—O1	121.32 (15)
C4—C5—C6	120.52 (13)	N3—C14—C15	115.37 (14)
C4—C5—H5	119.739	O1—C14—C15	123.28 (16)
C6—C5—H5	119.74	C14—C15—H15a	109.471
C5—C6—C7	120.46 (13)	C14—C15—H15b	109.472
C5—C6—H6	119.768	C14—C15—H15c	109.5 (7)
C7—C6—H6	119.769	H15a—C15—H15b	109.472
N2—C7—C6	119.07 (13)	H15a—C15—H15c	109.471
N2—C7—H7	120.466	H15b—C15—H15c	109.47
C6—C7—H7	120.465		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*n*···N1^{i}	0.880 (12)	2.162 (12)	3.0219 (16)	165.4 (13)

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