

2-[4,5-Diphenyl-2-(pyridin-4-yl)-1H-imidazol-1-yl]-ethanol

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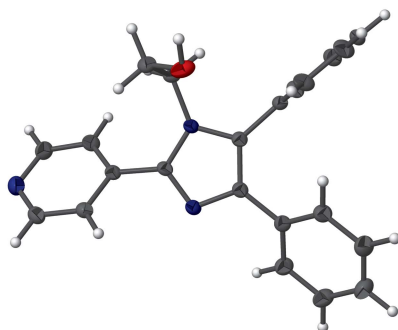
Keywords: crystal structure; imidazole; hydrogen bond; multi-component reactions.

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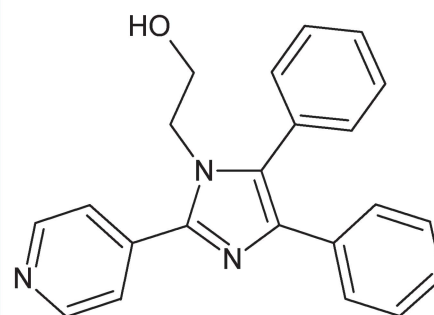
Structural data: full structural data are available from iucrdata.iucr.org

The basic building blocks of the three-dimensional structure of the title compound, C₂₂H₁₉N₃O, are helical chains running along the [101] direction and formed by O—H···N hydrogen bonds. C—H···O hydrogen bonds between chains generate sheets which are then joined together by C—H···N hydrogen bonds. The two- and three-dimensional structures also feature two sets of C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Imidazole derivatives have intensive synthetic interest due to their important biological activities, and many of these compounds are candidates for drug development (Romero *et al.*, 2014). On the other hand, the chemistry of imidazole and its pharmacological actions have attracted many chemists and biologists (Kumar, 2010; Shalini *et al.*, 2010; Bhatnagar *et al.*, 2011). In this context we report here the synthesis and crystal structure of the title compound.

In the title molecule (Fig. 1), the 4-pyridyl ring makes a dihedral angle of 36.43 (9)° with the imidazole ring. The dihedral angles between the imidazole and the C9–C14 and C15–C20 rings are, respectively, 81.98 (5) and 37.94 (6)°.

In the crystal, molecules form helical chains running parallel to [101] through O1—H1···N2ⁱ hydrogen bonds (Table 1). These chains are linked into sheets parallel to (101) by C5—H5···O1ⁱⁱ hydrogen bonds and the sheets are further associated into a three-dimensional layer structure through C13—H13···N3ⁱⁱⁱ hydrogen bonds (Table 1 and Figs.

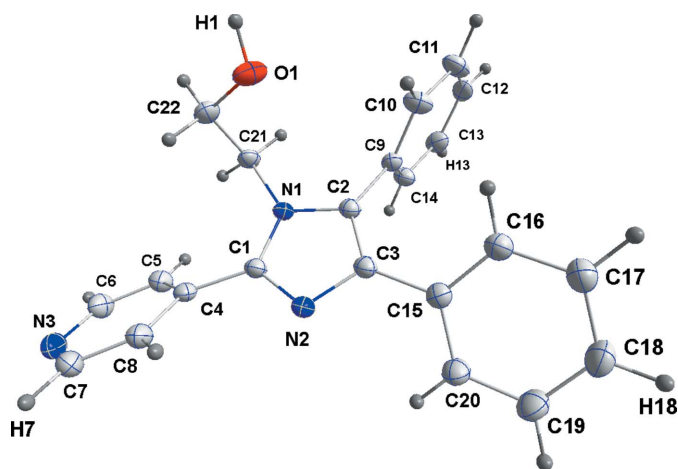


Figure 1
The title molecule, showing the atom-labeling scheme and 50% probability displacement ellipsoids.

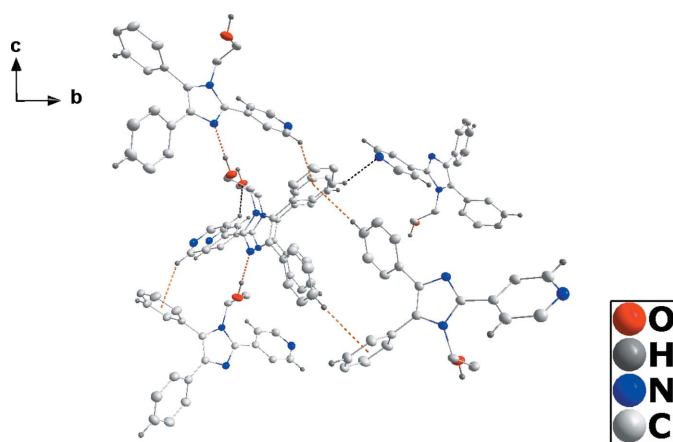


Figure 2
Detail of the intermolecular interactions, with O—H...N and C—H...N hydrogen bonds shown, respectively, as red and blue dotted lines. The C—H... π (ring) interactions are shown as orange dotted lines.

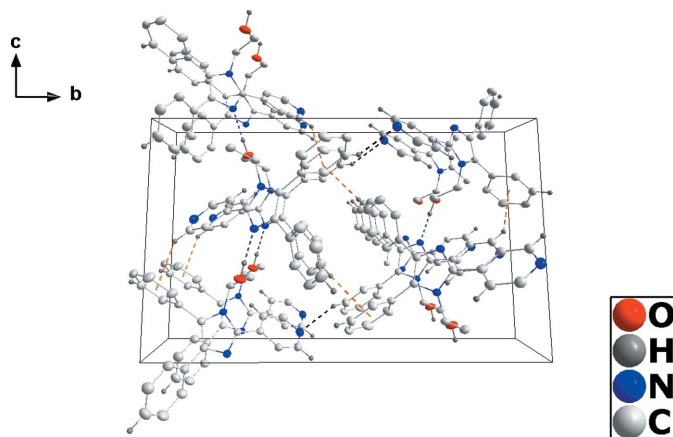


Figure 3
Packing viewed along the *a* axis, with intermolecular interactions shown as in Fig. 2.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

*Cg*1 is the centroid of the C9–C14 phenyl ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...N2 ⁱ	0.94 (2)	1.85 (2)	2.7857 (16)	169.4 (19)
C5—H5...O1 ⁱⁱ	0.992 (19)	2.448 (19)	3.2194 (18)	134.3 (14)
C13—H13...N3 ⁱⁱⁱ	0.99 (2)	2.52 (2)	3.327 (2)	138.0 (15)
C7—H7... <i>Cg</i> 1 ^{iv}	0.993 (18)	2.73 (2)	3.588 (2)	145 (1)
C18—H18... <i>Cg</i> 1 ^v	0.98 (2)	2.93 (2)	3.828 (2)	153 (1)

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x - 1, y, z$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$; (v) $-x + 2, -y + 1, -z + 1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}$
M_r	341.40
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (\AA)	5.7619 (2), 22.1304 (6), 13.6271 (4)
β ($^\circ$)	99.102 (1)
<i>V</i> (\AA^3)	1715.75 (9)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm^{-1})	0.66
Crystal size (mm)	0.19 \times 0.06 \times 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)
T_{min} , T_{max}	0.89, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13033, 3311, 2771
R_{int}	0.043
$(\sin \theta/\lambda)_{\text{max}}$ (\AA^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.038, 0.090, 1.05
No. of reflections	3311
No. of parameters	312
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e \AA^{-3})	0.20, -0.20

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

2 and 3). The two- and three-dimensional structures also feature two sets of C—H... π (ring) interactions (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

Benzil (1.06 g; 5 mmol), 4-pyridaldehyde (535 mg, 5 mmol), ammonium acetate (390 mg, 5 mmol) and monoethanolamine (305 mg, 5 mmol) were added to diethyl ammonium hydrogen sulfate (0.342 g, 2 mmol) in an oil bath at room temperature. The resulting mixture was heated at 373 K for an appropriate time. The reaction was monitored by TLC until completion, then washed with water. The resulting solid product was purified by recrystallization from ethanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170132 [<https://doi.org/10.1107/S2414314617001328>]

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2-[4,5-Diphenyl-2-(pyridin-4-yl)-1*H*-imidazol-1-yl]ethanol*Crystal data*

$C_{22}H_{19}N_3O$

$M_r = 341.40$

Monoclinic, $P2_1/n$

$a = 5.7619$ (2) Å

$b = 22.1304$ (6) Å

$c = 13.6271$ (4) Å

$\beta = 99.102$ (1)°

$V = 1715.75$ (9) Å³

$Z = 4$

$F(000) = 720$

$D_x = 1.322$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 8994 reflections

$\theta = 3.9$ – 72.4 °

$\mu = 0.66$ mm⁻¹

$T = 150$ K

Plate, colourless

$0.19 \times 0.06 \times 0.02$ mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS
diffractometer

Radiation source: INCOATEC I μ S micro-focus
source

Mirror monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2016)

$T_{\min} = 0.89$, $T_{\max} = 0.99$

13033 measured reflections

3311 independent reflections

2771 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\max} = 72.4$ °, $\theta_{\min} = 3.9$ °

$h = -7 \rightarrow 6$

$k = -27 \rightarrow 27$

$l = -14 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.090$

$S = 1.05$

3311 reflections

312 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.6309P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.20$ e Å⁻³

$\Delta\rho_{\min} = -0.20$ e Å⁻³

Extinction correction: *SHELXL2014* (Sheldrick,
2015), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0046 (4)

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.

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.87239 (19)	0.24860 (5)	0.84508 (8)	0.0303 (3)
H1	0.950 (4)	0.2368 (9)	0.9083 (17)	0.047 (6)*
N1	0.5090 (2)	0.30083 (5)	0.69732 (8)	0.0191 (3)
N2	0.5459 (2)	0.28733 (5)	0.53872 (8)	0.0205 (3)
N3	-0.0316 (2)	0.11711 (6)	0.57069 (10)	0.0293 (3)
C1	0.4465 (2)	0.26669 (6)	0.61350 (10)	0.0194 (3)
C2	0.6600 (2)	0.34551 (6)	0.67341 (10)	0.0193 (3)
C3	0.6802 (2)	0.33646 (6)	0.57505 (10)	0.0203 (3)
C4	0.2844 (2)	0.21494 (6)	0.60331 (10)	0.0199 (3)
C5	0.0828 (3)	0.21276 (7)	0.64771 (11)	0.0245 (3)
H5	0.038 (3)	0.2457 (8)	0.6905 (14)	0.036 (5)*
C6	-0.0644 (3)	0.16325 (7)	0.63044 (12)	0.0284 (3)
H6	-0.205 (3)	0.1610 (7)	0.6626 (13)	0.027 (4)*
C7	0.1622 (3)	0.12002 (7)	0.52763 (11)	0.0266 (3)
H7	0.193 (3)	0.0858 (8)	0.4844 (14)	0.033 (5)*
C8	0.3235 (3)	0.16674 (6)	0.54193 (11)	0.0231 (3)
H8	0.461 (3)	0.1664 (8)	0.5087 (14)	0.035 (5)*
C9	0.7402 (2)	0.39592 (6)	0.74245 (10)	0.0199 (3)
C10	0.9638 (3)	0.39745 (7)	0.79861 (11)	0.0273 (3)
H10	1.072 (3)	0.3620 (9)	0.7949 (14)	0.040 (5)*
C11	1.0354 (3)	0.44658 (8)	0.85989 (12)	0.0314 (4)
H11	1.194 (4)	0.4466 (9)	0.8994 (14)	0.041 (5)*
C12	0.8828 (3)	0.49414 (7)	0.86600 (11)	0.0279 (3)
H12	0.933 (3)	0.5292 (8)	0.9085 (14)	0.034 (5)*
C13	0.6582 (3)	0.49243 (7)	0.81202 (11)	0.0287 (3)
H13	0.549 (3)	0.5263 (9)	0.8187 (15)	0.041 (5)*
C14	0.5882 (3)	0.44385 (7)	0.75022 (11)	0.0247 (3)
H14	0.438 (3)	0.4424 (8)	0.7109 (14)	0.036 (5)*
C15	0.8124 (2)	0.37184 (6)	0.51075 (11)	0.0217 (3)
C16	1.0341 (3)	0.39503 (7)	0.54713 (12)	0.0279 (3)
H16	1.111 (3)	0.3872 (8)	0.6190 (15)	0.038 (5)*
C17	1.1579 (3)	0.42864 (8)	0.48648 (13)	0.0339 (4)
H17	1.320 (4)	0.4451 (9)	0.5137 (15)	0.048 (6)*
C18	1.0623 (3)	0.43897 (8)	0.38833 (13)	0.0346 (4)
H18	1.151 (3)	0.4626 (9)	0.3462 (14)	0.041 (5)*

C19	0.8441 (3)	0.41520 (8)	0.35077 (12)	0.0327 (4)
H19	0.775 (4)	0.4217 (9)	0.2804 (16)	0.050 (6)*
C20	0.7190 (3)	0.38220 (7)	0.41117 (11)	0.0273 (3)
H20	0.564 (3)	0.3656 (9)	0.3850 (14)	0.038 (5)*
C21	0.4766 (2)	0.28527 (7)	0.79934 (10)	0.0216 (3)
H21A	0.516 (3)	0.3223 (8)	0.8409 (13)	0.030 (4)*
H21B	0.312 (3)	0.2750 (8)	0.8021 (13)	0.031 (4)*
C22	0.6319 (3)	0.23327 (7)	0.84114 (11)	0.0261 (3)
H22A	0.592 (3)	0.2235 (8)	0.9102 (13)	0.030 (4)*
H22B	0.592 (3)	0.1977 (8)	0.7982 (13)	0.031 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0274 (5)	0.0430 (7)	0.0204 (6)	0.0062 (5)	0.0038 (4)	0.0075 (5)
N1	0.0212 (6)	0.0200 (6)	0.0154 (6)	-0.0010 (5)	0.0011 (4)	-0.0012 (4)
N2	0.0215 (6)	0.0217 (6)	0.0175 (6)	-0.0019 (5)	0.0009 (4)	-0.0012 (4)
N3	0.0306 (7)	0.0267 (7)	0.0294 (7)	-0.0049 (5)	0.0015 (5)	0.0018 (5)
C1	0.0207 (7)	0.0202 (7)	0.0163 (7)	0.0000 (5)	0.0000 (5)	-0.0018 (5)
C2	0.0185 (6)	0.0207 (7)	0.0179 (7)	0.0003 (5)	0.0004 (5)	0.0001 (5)
C3	0.0203 (7)	0.0206 (7)	0.0190 (7)	0.0001 (5)	0.0004 (5)	-0.0004 (5)
C4	0.0207 (7)	0.0214 (7)	0.0160 (7)	0.0003 (5)	-0.0013 (5)	0.0007 (5)
C5	0.0233 (7)	0.0268 (8)	0.0232 (8)	0.0012 (6)	0.0024 (6)	-0.0019 (6)
C6	0.0238 (7)	0.0329 (8)	0.0287 (8)	-0.0036 (6)	0.0045 (6)	0.0009 (6)
C7	0.0315 (8)	0.0231 (7)	0.0239 (8)	-0.0012 (6)	0.0005 (6)	-0.0014 (6)
C8	0.0247 (7)	0.0247 (7)	0.0197 (7)	-0.0008 (6)	0.0023 (6)	-0.0008 (5)
C9	0.0218 (7)	0.0220 (7)	0.0157 (7)	-0.0022 (5)	0.0024 (5)	-0.0003 (5)
C10	0.0237 (7)	0.0338 (8)	0.0232 (8)	0.0023 (6)	-0.0003 (6)	-0.0059 (6)
C11	0.0245 (8)	0.0421 (9)	0.0256 (8)	-0.0064 (7)	-0.0021 (6)	-0.0081 (7)
C12	0.0385 (9)	0.0248 (8)	0.0199 (8)	-0.0100 (6)	0.0027 (6)	-0.0038 (6)
C13	0.0377 (9)	0.0218 (7)	0.0258 (8)	0.0032 (7)	0.0024 (6)	-0.0017 (6)
C14	0.0236 (7)	0.0253 (7)	0.0232 (8)	0.0005 (6)	-0.0022 (6)	-0.0019 (6)
C15	0.0226 (7)	0.0209 (7)	0.0216 (7)	0.0013 (5)	0.0036 (5)	-0.0002 (5)
C16	0.0267 (8)	0.0329 (8)	0.0236 (8)	-0.0047 (6)	0.0026 (6)	-0.0014 (6)
C17	0.0289 (8)	0.0396 (9)	0.0336 (9)	-0.0089 (7)	0.0068 (7)	-0.0011 (7)
C18	0.0360 (9)	0.0358 (9)	0.0344 (10)	-0.0050 (7)	0.0125 (7)	0.0068 (7)
C19	0.0345 (9)	0.0375 (9)	0.0260 (9)	0.0012 (7)	0.0042 (7)	0.0079 (7)
C20	0.0256 (8)	0.0319 (8)	0.0239 (8)	-0.0009 (6)	0.0018 (6)	0.0032 (6)
C21	0.0239 (7)	0.0265 (7)	0.0145 (7)	-0.0023 (6)	0.0035 (5)	-0.0015 (5)
C22	0.0307 (8)	0.0281 (8)	0.0190 (8)	-0.0017 (6)	0.0024 (6)	0.0032 (6)

Geometric parameters (Å, °)

O1—C22	1.4191 (19)	C10—H10	1.009 (19)
O1—H1	0.94 (2)	C11—C12	1.382 (2)
N1—C1	1.3693 (17)	C11—H11	0.98 (2)
N1—C2	1.3894 (17)	C12—C13	1.384 (2)
N1—C21	1.4726 (18)	C12—H12	0.984 (19)

N2—C1	1.3267 (18)	C13—C14	1.386 (2)
N2—C3	1.3799 (17)	C13—H13	0.99 (2)
N3—C6	1.338 (2)	C14—H14	0.94 (2)
N3—C7	1.342 (2)	C15—C16	1.393 (2)
C1—C4	1.4703 (19)	C15—C20	1.397 (2)
C2—C3	1.378 (2)	C16—C17	1.390 (2)
C2—C9	1.4851 (19)	C16—H16	1.02 (2)
C3—C15	1.4740 (19)	C17—C18	1.383 (2)
C4—C5	1.393 (2)	C17—H17	1.02 (2)
C4—C8	1.3956 (19)	C18—C19	1.384 (2)
C5—C6	1.383 (2)	C18—H18	0.98 (2)
C5—H5	0.992 (19)	C19—C20	1.385 (2)
C6—H6	0.982 (17)	C19—H19	0.99 (2)
C7—C8	1.383 (2)	C20—H20	0.980 (19)
C7—H7	0.993 (18)	C21—C22	1.513 (2)
C8—H8	0.975 (19)	C21—H21A	1.001 (18)
C9—C14	1.390 (2)	C21—H21B	0.982 (18)
C9—C10	1.391 (2)	C22—H22A	1.028 (18)
C10—C11	1.393 (2)	C22—H22B	0.986 (18)
C22—O1—H1	106.5 (13)	C11—C12—C13	119.82 (14)
C1—N1—C2	106.80 (11)	C11—C12—H12	120.4 (11)
C1—N1—C21	127.05 (11)	C13—C12—H12	119.8 (11)
C2—N1—C21	124.43 (11)	C12—C13—C14	120.12 (14)
C1—N2—C3	106.34 (11)	C12—C13—H13	118.9 (12)
C6—N3—C7	115.92 (13)	C14—C13—H13	121.0 (12)
N2—C1—N1	111.23 (12)	C13—C14—C9	120.80 (14)
N2—C1—C4	122.72 (12)	C13—C14—H14	121.5 (11)
N1—C1—C4	126.01 (12)	C9—C14—H14	117.7 (11)
C3—C2—N1	106.07 (12)	C16—C15—C20	118.40 (14)
C3—C2—C9	131.28 (13)	C16—C15—C3	121.02 (13)
N1—C2—C9	121.97 (12)	C20—C15—C3	120.57 (13)
C2—C3—N2	109.56 (12)	C17—C16—C15	120.90 (15)
C2—C3—C15	129.19 (13)	C17—C16—H16	118.3 (11)
N2—C3—C15	121.22 (12)	C15—C16—H16	120.8 (11)
C5—C4—C8	117.29 (13)	C18—C17—C16	120.03 (15)
C5—C4—C1	123.16 (13)	C18—C17—H17	119.7 (12)
C8—C4—C1	119.45 (12)	C16—C17—H17	120.3 (12)
C6—C5—C4	119.00 (14)	C17—C18—C19	119.63 (15)
C6—C5—H5	118.3 (11)	C17—C18—H18	119.4 (12)
C4—C5—H5	122.7 (11)	C19—C18—H18	121.0 (11)
N3—C6—C5	124.48 (14)	C18—C19—C20	120.54 (15)
N3—C6—H6	116.0 (10)	C18—C19—H19	120.5 (12)
C5—C6—H6	119.5 (10)	C20—C19—H19	119.0 (12)
N3—C7—C8	124.12 (14)	C19—C20—C15	120.48 (14)
N3—C7—H7	117.7 (10)	C19—C20—H20	120.8 (11)
C8—C7—H7	118.2 (10)	C15—C20—H20	118.8 (11)
C7—C8—C4	119.16 (13)	N1—C21—C22	112.19 (12)

C7—C8—H8	120.5 (11)	N1—C21—H21A	107.0 (10)
C4—C8—H8	120.3 (11)	C22—C21—H21A	110.0 (10)
C14—C9—C10	118.64 (13)	N1—C21—H21B	111.0 (10)
C14—C9—C2	119.02 (12)	C22—C21—H21B	109.1 (10)
C10—C9—C2	122.34 (13)	H21A—C21—H21B	107.5 (14)
C9—C10—C11	120.64 (14)	O1—C22—C21	110.38 (12)
C9—C10—H10	118.7 (11)	O1—C22—H22A	112.1 (10)
C11—C10—H10	120.7 (11)	C21—C22—H22A	107.4 (10)
C12—C11—C10	119.95 (14)	O1—C22—H22B	110.4 (10)
C12—C11—H11	120.7 (11)	C21—C22—H22B	108.3 (10)
C10—C11—H11	119.3 (11)	H22A—C22—H22B	108.1 (14)
C3—N2—C1—N1	0.56 (15)	C3—C2—C9—C14	91.39 (19)
C3—N2—C1—C4	178.53 (12)	N1—C2—C9—C14	-77.78 (17)
C2—N1—C1—N2	-0.68 (15)	C3—C2—C9—C10	-87.5 (2)
C21—N1—C1—N2	-166.12 (12)	N1—C2—C9—C10	103.31 (17)
C2—N1—C1—C4	-178.58 (13)	C14—C9—C10—C11	-1.2 (2)
C21—N1—C1—C4	16.0 (2)	C2—C9—C10—C11	177.67 (14)
C1—N1—C2—C3	0.51 (14)	C9—C10—C11—C12	0.6 (2)
C21—N1—C2—C3	166.43 (12)	C10—C11—C12—C13	0.7 (2)
C1—N1—C2—C9	172.07 (12)	C11—C12—C13—C14	-1.5 (2)
C21—N1—C2—C9	-22.0 (2)	C12—C13—C14—C9	0.9 (2)
N1—C2—C3—N2	-0.19 (15)	C10—C9—C14—C13	0.5 (2)
C9—C2—C3—N2	-170.65 (13)	C2—C9—C14—C13	-178.47 (14)
N1—C2—C3—C15	177.92 (13)	C2—C3—C15—C16	39.6 (2)
C9—C2—C3—C15	7.5 (2)	N2—C3—C15—C16	-142.47 (14)
C1—N2—C3—C2	-0.22 (15)	C2—C3—C15—C20	-141.27 (15)
C1—N2—C3—C15	-178.51 (12)	N2—C3—C15—C20	36.6 (2)
N2—C1—C4—C5	-140.18 (14)	C20—C15—C16—C17	1.2 (2)
N1—C1—C4—C5	37.5 (2)	C3—C15—C16—C17	-179.66 (14)
N2—C1—C4—C8	35.95 (19)	C15—C16—C17—C18	-0.6 (3)
N1—C1—C4—C8	-146.38 (14)	C16—C17—C18—C19	-0.6 (3)
C8—C4—C5—C6	1.1 (2)	C17—C18—C19—C20	1.2 (3)
C1—C4—C5—C6	177.27 (13)	C18—C19—C20—C15	-0.7 (3)
C7—N3—C6—C5	1.5 (2)	C16—C15—C20—C19	-0.5 (2)
C4—C5—C6—N3	-2.2 (2)	C3—C15—C20—C19	-179.69 (14)
C6—N3—C7—C8	0.2 (2)	C1—N1—C21—C22	68.45 (17)
N3—C7—C8—C4	-1.1 (2)	C2—N1—C21—C22	-94.58 (15)
C5—C4—C8—C7	0.5 (2)	N1—C21—C22—O1	61.03 (16)
C1—C4—C8—C7	-175.89 (13)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 is the centroid of the C9–C14 phenyl ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N2 ⁱ	0.94 (2)	1.85 (2)	2.7857 (16)	169.4 (19)
C5—H5 \cdots O1 ⁱⁱ	0.992 (19)	2.448 (19)	3.2194 (18)	134.3 (14)
C13—H13 \cdots N3 ⁱⁱⁱ	0.99 (2)	2.52 (2)	3.327 (2)	138.0 (15)

C7—H7...Cg1 ^{iv}	0.993 (18)	2.73 (2)	3.588 (2)	145 (1)
C18—H18...Cg1 ^v	0.98 (2)	2.93 (2)	3.828 (2)	153 (1)

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $x-1, y, z$; (iii) $-x+1/2, y+1/2, -z+3/2$; (iv) $x-1/2, -y+1/2, z-1/2$; (v) $-x+2, -y+1, -z+1$.