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N-(*tert*-Butyl)-2-(2-nitrophenyl)imidazo[1,2-*a*]-pyridin-3-amine

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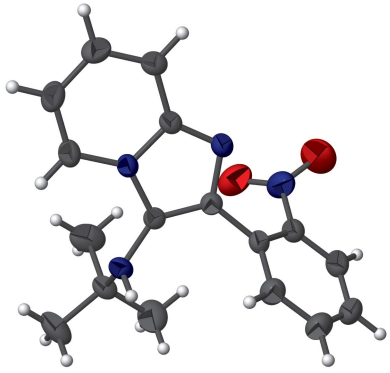
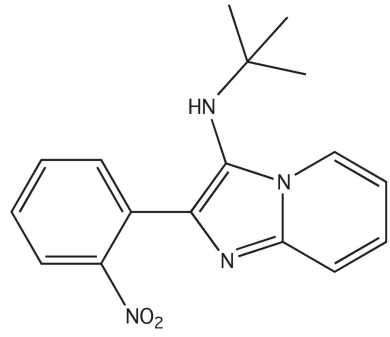
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{18}N_4O_2$, the dihedral angle between the pyridine and benzene rings is 55.68 (11)°. In the crystal, N—H···N hydrogen bonds link the molecules into [010] chains.

3D view



Chemical scheme



Structure description

Imidazoles are heterocyclic compounds that show important pharmacological and biochemical properties including anti-fungal (Banfi, *et al.*, 2006), anti-bacterial (Jackson *et al.*, 2000), anti-tumour (Dooley *et al.*, 1992; Cui *et al.*, 2003), anti-protozoal (Biftu *et al.*, 2006), anti-herpes (Gudmundsson *et al.*, 2007), anti-inflammatory (Rupert *et al.*, 2003), anti-ulcerative, anti-hypertensive, anti-histaminic and anti-helminthic properties (Spasov *et al.*, 1999). These compounds are highly active against human cytomegalovirus and varicella-zoster virus (Gueiffier *et al.*,1998). In a continuation of our studies on imdiazole derivatives (Dhanalakshmi *et al.*, 2018; Mala *et al.*, 2019), we herein report the synthesis and crystal structure analysis of the title compound.

The title compound (Fig. 1) consists of imidazole, pyridine and benzene rings with a nitro group connected at the C9 position of the benzene ring and an N-bonded *tert*-butyl group (N3/C15–C18) connected at C6 of the imidazole ring. The pyridine ring (C1–C5/N1) is fused to the imidazole ring at a dihedral angle of 0.76 (9)°. The dihedral angle between the pyridine and benzene rings is 55.68 (11)°. The dihedral angle between the NO_2 group (N4/O1/O2) and the benzene ring is 49 (3)°. In the crystal, molecules are linked by N3—H3*A*···N2 hydrogen bonds (Table 1) as shown in Fig. 2.

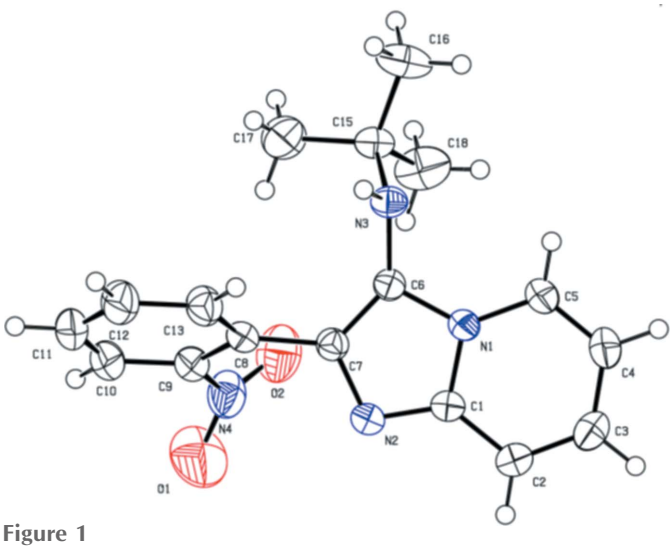


Figure 1
Asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Synthesis and crystallization

N-(*tert*-Butyl)-2-(2-nitrophenyl)imidazo[1,2-*a*]pyridin-3-amine was prepared by our reported method (reagent quantities: 1 eq. of *tert*-butyl isocyanide and 0.5 mmol of iodine; Dhanalakshmi *et al.*, 2018) and confirmed by NMR, ESI–MS and IR spectroscopy. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.19 (*d*, *J* = 6.9, 1H), 7.91 (*dd*, *J* = 8.1, 0.9, 1H), 7.80 (*d*, *J* = 1.2, 1H), 7.65 (*d*, *J* = 1.1, 1H), 7.51 (*dd*, *J* = 16.4, 4.9, 2H), 7.16 (*ddd*, *J* = 9.0, 6.7, 1.2, 1H), 6.81 (*d*, *J* = 0.9, 1H), 0.95 (*s*, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.51, 147.62, 142.42, 137.93, 136.20, 132.85, 132.39, 130.30, 128.38, 124.69, 124.37, 124.25, 123.33, 117.72, 113.94, 111.77, 108.78, 55.60, 30.05. Chemical formula: $C_{17}H_{18}N_4O_2$ expected or exact mass 310.1430. Obtained mass: 3110.20 *m*/*z*.

Refinement

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

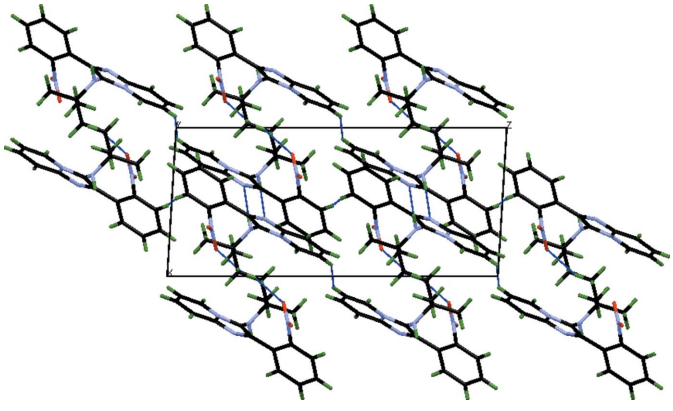


Figure 2
Packing of the molecules of the title compound. Hydrogen bonds are shown as blue lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N2^{i}	0.85 (2)	2.29 (2)	3.112 (3)	164 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}N_4O_2$
M_r	310.35
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	8.046 (7), 11.038 (10), 17.912 (15)
β (°)	93.47 (3)
V (Å^3)	1588 (2)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa *APEX2* CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.678, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27960, 2770, 2430
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.048, 0.133, 1.06
No. of reflections	2770
No. of parameters	212
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.20

Computer programs: *APEX3*, *SAINT* and *XPREP* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

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Crystal data

$C_{17}H_{18}N_4O_2$
M_r = 310.35
Monoclinic, $P2_1/c$
a = 8.046 (7) Å
b = 11.038 (10) Å
c = 17.912 (15) Å
β = 93.47 (3)°
V = 1588 (2) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.298 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9919 reflections
θ = 2.9–30.5°
μ = 0.09 mm^{-1}
T = 296 K
Block, brown
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEX2 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.678, T_{max} = 0.746
27960 measured reflections
2770 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.0°, θ_{min} = 2.9°
h = −9→9
k = −13→13
l = −21→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.133
S = 1.06
2770 reflections
212 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.9086P]$ 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}

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	0.30330 (19)	0.23121 (15)	0.15414 (9)	0.0301 (4)
C2	0.2519 (2)	0.17506 (17)	0.08591 (10)	0.0379 (4)
H2	0.274952	0.093657	0.078025	0.045*
C3	0.1687 (3)	0.24088 (19)	0.03207 (10)	0.0459 (5)
H3	0.133177	0.204120	−0.012811	0.055*
C4	0.1353 (3)	0.36484 (19)	0.04332 (11)	0.0486 (5)
H4	0.077691	0.408864	0.005807	0.058*
C5	0.1860 (2)	0.42014 (17)	0.10783 (10)	0.0394 (4)
H5	0.164764	0.502022	0.114921	0.047*
C6	0.33523 (19)	0.38898 (14)	0.23310 (9)	0.0279 (4)
C7	0.40432 (19)	0.28449 (15)	0.26309 (9)	0.0299 (4)
C8	0.4982 (2)	0.26944 (15)	0.33571 (9)	0.0326 (4)
C9	0.4610 (2)	0.18049 (16)	0.38715 (10)	0.0387 (4)
C10	0.5537 (3)	0.16271 (18)	0.45377 (11)	0.0493 (5)
H10	0.524721	0.102488	0.486886	0.059*
C11	0.6900 (3)	0.2359 (2)	0.47024 (12)	0.0534 (6)
H11	0.753904	0.225574	0.514800	0.064*
C12	0.7309 (3)	0.3245 (2)	0.42035 (13)	0.0535 (5)
H12	0.823182	0.373485	0.431392	0.064*
C13	0.6367 (2)	0.34146 (18)	0.35419 (11)	0.0425 (4)
H13	0.666250	0.402001	0.321398	0.051*
C15	0.1893 (2)	0.54261 (15)	0.30802 (10)	0.0355 (4)
C16	0.1656 (3)	0.67880 (18)	0.30153 (14)	0.0581 (6)
H16A	0.083002	0.704460	0.334670	0.087*
H16B	0.269065	0.718842	0.314819	0.087*
H16C	0.129591	0.699179	0.251009	0.087*
C17	0.2453 (3)	0.5097 (2)	0.38823 (12)	0.0607 (6)
H17A	0.160266	0.532130	0.420949	0.091*
H17B	0.264531	0.423958	0.391680	0.091*
H17C	0.346312	0.552144	0.402593	0.091*
C18	0.0280 (3)	0.4774 (2)	0.28534 (15)	0.0605 (6)
H18A	−0.055408	0.498849	0.319132	0.091*
H18B	−0.008882	0.500645	0.235408	0.091*
H18C	0.046138	0.391461	0.287147	0.091*
N1	0.26936 (16)	0.35359 (12)	0.16279 (7)	0.0289 (3)
N2	0.38504 (17)	0.18709 (13)	0.21493 (8)	0.0334 (3)
N3	0.31833 (18)	0.50905 (12)	0.25542 (8)	0.0315 (3)
N4	0.3144 (2)	0.10426 (16)	0.37388 (10)	0.0530 (5)
O1	0.3307 (3)	−0.00446 (17)	0.38458 (14)	0.1032 (8)
O2	0.1814 (2)	0.15316 (18)	0.35684 (9)	0.0685 (5)
H3A	0.410 (3)	0.544 (2)	0.2658 (12)	0.045 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0304 (8)	0.0275 (8)	0.0324 (9)	0.0014 (6)	0.0033 (6)	−0.0013 (7)
C2	0.0429 (10)	0.0343 (9)	0.0364 (9)	0.0015 (7)	0.0011 (8)	−0.0052 (7)
C3	0.0528 (11)	0.0516 (12)	0.0324 (9)	0.0022 (9)	−0.0032 (8)	−0.0083 (8)
C4	0.0586 (12)	0.0519 (12)	0.0340 (10)	0.0139 (10)	−0.0082 (8)	0.0040 (8)
C5	0.0485 (10)	0.0346 (9)	0.0346 (9)	0.0094 (8)	−0.0014 (8)	0.0040 (7)
C6	0.0286 (8)	0.0269 (8)	0.0281 (8)	−0.0014 (6)	0.0018 (6)	0.0008 (6)
C7	0.0291 (8)	0.0295 (9)	0.0308 (8)	−0.0001 (6)	0.0006 (6)	0.0002 (6)
C8	0.0344 (8)	0.0287 (8)	0.0341 (9)	0.0065 (7)	−0.0019 (7)	−0.0011 (7)
C9	0.0457 (10)	0.0325 (9)	0.0371 (9)	0.0030 (8)	−0.0037 (8)	0.0005 (7)
C10	0.0678 (13)	0.0388 (10)	0.0398 (10)	0.0066 (9)	−0.0090 (9)	0.0062 (8)
C11	0.0628 (13)	0.0491 (12)	0.0454 (11)	0.0098 (10)	−0.0210 (10)	−0.0016 (9)
C12	0.0480 (11)	0.0521 (12)	0.0577 (13)	−0.0014 (9)	−0.0179 (10)	−0.0033 (10)
C13	0.0407 (10)	0.0409 (10)	0.0448 (11)	−0.0020 (8)	−0.0051 (8)	0.0026 (8)
C15	0.0380 (9)	0.0287 (9)	0.0405 (10)	0.0012 (7)	0.0089 (7)	−0.0022 (7)
C16	0.0647 (14)	0.0332 (11)	0.0792 (16)	0.0088 (9)	0.0255 (12)	−0.0001 (10)
C17	0.0765 (16)	0.0661 (15)	0.0409 (11)	0.0157 (12)	0.0149 (11)	−0.0004 (10)
C18	0.0394 (11)	0.0638 (14)	0.0799 (16)	−0.0092 (10)	0.0179 (11)	−0.0181 (12)
N1	0.0311 (7)	0.0266 (7)	0.0290 (7)	0.0024 (5)	0.0013 (5)	0.0015 (5)
N2	0.0369 (8)	0.0288 (7)	0.0342 (8)	0.0045 (6)	−0.0004 (6)	−0.0007 (6)
N3	0.0318 (8)	0.0258 (7)	0.0372 (8)	−0.0029 (6)	0.0040 (6)	−0.0021 (6)
N4	0.0664 (12)	0.0468 (11)	0.0445 (10)	−0.0142 (9)	−0.0074 (8)	0.0111 (8)
O1	0.1304 (19)	0.0502 (11)	0.1245 (19)	−0.0298 (11)	−0.0298 (15)	0.0251 (11)
O2	0.0582 (10)	0.0850 (13)	0.0613 (10)	−0.0176 (9)	−0.0049 (8)	0.0064 (9)

Geometric parameters (Å, º)

C1—N2	1.330 (2)	C11—C12	1.378 (3)
C1—N1	1.389 (2)	C11—H11	0.9300
C1—C2	1.410 (3)	C12—C13	1.380 (3)
C2—C3	1.352 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.411 (3)	C15—N3	1.490 (2)
C3—H3	0.9300	C15—C18	1.518 (3)
C4—C5	1.348 (3)	C15—C16	1.519 (3)
C4—H4	0.9300	C15—C17	1.523 (3)
C5—N1	1.371 (2)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—C7	1.375 (2)	C16—H16C	0.9600
C6—N1	1.392 (2)	C17—H17A	0.9600
C6—N3	1.393 (2)	C17—H17B	0.9600
C7—N2	1.381 (2)	C17—H17C	0.9600
C7—C8	1.473 (2)	C18—H18A	0.9600
C8—C9	1.391 (3)	C18—H18B	0.9600
C8—C13	1.392 (3)	C18—H18C	0.9600
C9—C10	1.382 (3)	N3—H3A	0.85 (2)

C9—N4	1.457 (3)	N4—O2	1.221 (3)
C10—C11	1.380 (3)	N4—O1	1.221 (3)
C10—H10	0.9300		

N2—C1—N1	110.84 (14)	C12—C13—H13	119.4
N2—C1—C2	130.80 (16)	C8—C13—H13	119.4
N1—C1—C2	118.36 (15)	N3—C15—C18	109.28 (16)
C3—C2—C1	119.26 (18)	N3—C15—C16	106.68 (15)
C3—C2—H2	120.4	C18—C15—C16	110.31 (18)
C1—C2—H2	120.4	N3—C15—C17	111.07 (16)
C2—C3—C4	120.63 (18)	C18—C15—C17	109.77 (18)
C2—C3—H3	119.7	C16—C15—C17	109.69 (18)
C4—C3—H3	119.7	C15—C16—H16A	109.5
C5—C4—C3	120.74 (17)	C15—C16—H16B	109.5
C5—C4—H4	119.6	H16A—C16—H16B	109.5
C3—C4—H4	119.6	C15—C16—H16C	109.5
C4—C5—N1	118.85 (18)	H16A—C16—H16C	109.5
C4—C5—H5	120.6	H16B—C16—H16C	109.5
N1—C5—H5	120.6	C15—C17—H17A	109.5
C7—C6—N1	103.93 (14)	C15—C17—H17B	109.5
C7—C6—N3	136.86 (16)	H17A—C17—H17B	109.5
N1—C6—N3	119.21 (14)	C15—C17—H17C	109.5
C6—C7—N2	112.41 (15)	H17A—C17—H17C	109.5
C6—C7—C8	127.80 (15)	H17B—C17—H17C	109.5
N2—C7—C8	119.72 (15)	C15—C18—H18A	109.5
C9—C8—C13	116.53 (16)	C15—C18—H18B	109.5
C9—C8—C7	123.01 (16)	H18A—C18—H18B	109.5
C13—C8—C7	120.37 (16)	C15—C18—H18C	109.5
C10—C9—C8	123.05 (18)	H18A—C18—H18C	109.5
C10—C9—N4	116.62 (17)	H18B—C18—H18C	109.5
C8—C9—N4	120.27 (16)	C5—N1—C1	122.15 (15)
C11—C10—C9	118.80 (19)	C5—N1—C6	129.96 (15)
C11—C10—H10	120.6	C1—N1—C6	107.89 (13)
C9—C10—H10	120.6	C1—N2—C7	104.93 (14)
C12—C11—C10	119.67 (18)	C6—N3—C15	120.11 (14)
C12—C11—H11	120.2	C6—N3—H3A	113.4 (15)
C10—C11—H11	120.2	C15—N3—H3A	112.5 (15)
C11—C12—C13	120.8 (2)	O2—N4—O1	123.9 (2)
C11—C12—H12	119.6	O2—N4—C9	118.32 (18)
C13—C12—H12	119.6	O1—N4—C9	117.6 (2)
C12—C13—C8	121.11 (19)		

N2—C1—C2—C3	179.80 (18)	C4—C5—N1—C1	0.0 (3)
N1—C1—C2—C3	−1.4 (2)	C4—C5—N1—C6	179.30 (17)
C1—C2—C3—C4	0.8 (3)	N2—C1—N1—C5	−179.99 (15)
C2—C3—C4—C5	0.2 (3)	C2—C1—N1—C5	1.0 (2)
C3—C4—C5—N1	−0.6 (3)	N2—C1—N1—C6	0.59 (18)
N1—C6—C7—N2	0.24 (18)	C2—C1—N1—C6	−178.43 (14)

N3—C6—C7—N2	−179.97 (17)	C7—C6—N1—C5	−179.84 (16)
N1—C6—C7—C8	177.11 (15)	N3—C6—N1—C5	0.3 (2)
N3—C6—C7—C8	−3.1 (3)	C7—C6—N1—C1	−0.49 (16)
C6—C7—C8—C9	129.2 (2)	N3—C6—N1—C1	179.68 (14)
N2—C7—C8—C9	−54.2 (2)	N1—C1—N2—C7	−0.43 (17)
C6—C7—C8—C13	−54.4 (3)	C2—C1—N2—C7	178.44 (17)
N2—C7—C8—C13	122.28 (19)	C6—C7—N2—C1	0.11 (18)
C13—C8—C9—C10	0.4 (3)	C8—C7—N2—C1	−177.04 (14)
C7—C8—C9—C10	176.93 (17)	C7—C6—N3—C15	−77.9 (3)
C13—C8—C9—N4	177.47 (17)	N1—C6—N3—C15	101.86 (18)
C7—C8—C9—N4	−5.9 (3)	C18—C15—N3—C6	−43.1 (2)
C8—C9—C10—C11	−0.3 (3)	C16—C15—N3—C6	−162.30 (17)
N4—C9—C10—C11	−177.48 (19)	C17—C15—N3—C6	78.2 (2)
C9—C10—C11—C12	−0.1 (3)	C10—C9—N4—O2	128.0 (2)
C10—C11—C12—C13	0.4 (3)	C8—C9—N4—O2	−49.3 (3)
C11—C12—C13—C8	−0.3 (3)	C10—C9—N4—O1	−48.0 (3)
C9—C8—C13—C12	−0.1 (3)	C8—C9—N4—O1	134.7 (2)
C7—C8—C13—C12	−176.75 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N2^{i}	0.85 (2)	2.29 (2)	3.112 (3)	164 (2)

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