Acta Crystallographica Section E

**Structure Reports Online**

ISSN 1600-5368

# 1-(2,3,4,5,6-Pentamethylbenzyl)-2-(pyridin-2-yl)-1*H*-benzimidazole

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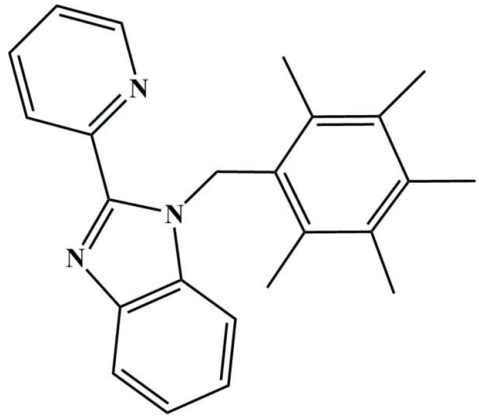
Received 28 March 2014; accepted 9 April 2014

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.052; $wR$ factor = 0.150; data-to-parameter ratio = 14.7.

In the title compound, $C_{24}H_{25}N_3$, the benzimidazole ring system is essentially planar, with an r.m.s. deviation of 0.017 Å, and forms dihedral angles of 7.81 (5) and 87.61 (4)° with the pyridine and benzene rings, respectively. An intramolecular C—H···N hydrogen bond is observed. In the crystal, molecules are stacked along the $a$ axis by weak C—H···$\pi$ interactions.

## Related literature

For the use of 2-(2-pyridyl)benzimidazole in coordination chemistry, see: Sahin *et al.* (2010); Harkins *et al.* (1956); Chiswell *et al.* (1964); De Castro *et al.* (1991); Maekawa *et al.* (1994); Khalil *et al.* (2001); Boca *et al.* (1997). For the use of N—N-type ligand systems involving 2,2′-bipyridine, see: Lippert (1999); Wong & Giandomenico (1999), Kelland & Farrell (2000). For related structures, see: Çelik *et al.* (2007, 2009, 2014).



## Experimental

### Crystal data

$C_{24}H_{25}N_3$
$M_r$ = 355.47
Monoclinic, $P2_1/n$
$a$ = 5.3470 (3) Å
$b$ = 21.0622 (12) Å
$c$ = 17.0379 (9) Å
$\beta$ = 97.699 (3)°
$V$ = 1901.50 (18) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 296 K
0.25 × 0.20 × 0.15 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
$T_{min}$ = 0.982, $T_{max}$ = 0.989
25354 measured reflections
3741 independent reflections
3056 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.150
$S$ = 1.04
3741 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

*Cg* is the centroid of the C7–C12 benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13$A$···$Cg^{i}$ | 0.97 | 2.91 | 3.6941 (18) | 139 |
| C13—H13$B$···N1 | 0.97 | 2.30 | 3.029 (2) | 131 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

The authors are indebted to the X-ray laboratory of Dicle University Science and the Technology Application and Research Center, Diyarbakir, Turkey, for use of the X-ray diffractometer.

Supporting information for this paper is available from the IUCr electronic archives (Reference: RZ5115).

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# supporting information

*Acta Cryst.* (2014). E**70**, o563–o564 [doi:10.1107/S1600536814007934]

## 1-(2,3,4,5,6-Pentamethylbenzyl)-2-(pyridin-2-yl)-1*H*-benzimidazole

**Fırat Anĝay, Ömer Çelik, Orhan Barlık and Mahmut Ulusoy**

### S1. Comment

The N—N type ligand system 2-(2-pyridyl)benzimidazole has a venerable history in coordination chemistry (Sahin *et al.*, 2010; Harkins *et al.*, 1956; Chiswell *et al.*, 1964; De Castro *et al.*, 1991; Maekawa *et al.*, 1994; Khalil *et al.*, 2001; Boca *et al.*, 1997). Lots of platinum chemistry bearing N—N type ligand systems involving 2,2′-bipyridine has been reported aimed at the design of drugs having less serious side-effects than those of cisplatin, or which could extend the scope of Pt based chemotherapy to tumours (Lippert, 1999; Wong & Giandomenico, 1999; Kelland & Farrell, 2000).

The molecular structure of the title compound is shown in Fig. 1. Bond lengths and angles are in good agreement with those reported for related structures (Çelik *et al.*, 2007; Çelik *et al.*, 2009; Çelik *et al.*, 2014). The benzimidazole ring system is substantially planar, the maximum deviation being 0.027 (2) Å for atom C8, and forms dihedral angles of 7.81 (5) and 87.61 (4)° with the mean planes through the pyridine (N1/C1–C5) and phenyl (C14–C19) rings, respectively. An intramolecular C—H···N hydrogen bond is present (Table 1). In the crystal structure (Fig. 2), molecules are stacked along the *a* axis by weak C—H···$\pi$ hydrogen interactions (Table 1) involving the C7—C12 benzene ring of the benzimidazole moiety.

### S2. Experimental

NaH (60%) (398 mg, 11.0 mmol) was washed two times with dry hexane, filtered off *via* cannula and a solution of the 2-pyridiylbenzimidazole (1.95 g, 10.0 mmol) in dry toluene (10 ml) was added, then the solution was heated at 90°C for 24 h. Evolution of hydrogen was observed at this temperature. 2,3,4,5,6-Pentamethylbenzyl bromide (2.45 g, 10.0 mmol) was added to this mixture at room temperature and then heated again at 90°C for 1 day. Then volatiles were evaporated in vacuum to dryness. The residue was dissolved in $CH_2C_{l2}$ and filtered *via* cannula on celite. The desired product was obtained after concentration of $CH_2C_{l2}$ (15 ml) and then precipitated with hexane (30 ml). The off-white solid obtained in 86% yield. M. p. 416–418 K. $^1$H NMR (400 MHz, $CDCl_3$, $\delta$ p.p.m.): 1.26 (s, 6H, *o*-$(CH_3)_2$); 1.36(s, 6H, *m*-$(CH_3)_2$); 2.13–2.20 (s, 3H, *p*-$CH_3$); 5.50 (s, 2H, N—$CH_2$); 6.86 (s, 1H, Ar—CH); 7.11 (s, 1H, Ar—CH); 7.26 (s, 1H, Ar—CH); 7.35 (s, 1H, Ar—CH); 7.49 (s, 1H, Ar—CH); 8.46 (s, 1H, Ar—CH); 10.19 (s, 2H, Ar—CH). $^{13}$C NMR (100.56 MHz, $CDCl_3$, $\delta$ p.p.m.): 17.0; 17.4; 29.6; 31.7; 34.4; 35.2; 48.7; 49.3; 56.2; 117.9; 121.2; 122.4; 125.5; 126.5; 133.8; 134.0; 137.5; 140.7; 158.0; 167.9.

### S3. Refinement

All H atoms were placed geometrically and refined using a riding model approximation, with C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(C) for methyl H atoms. A rotating group model was applied to the methyl groups.

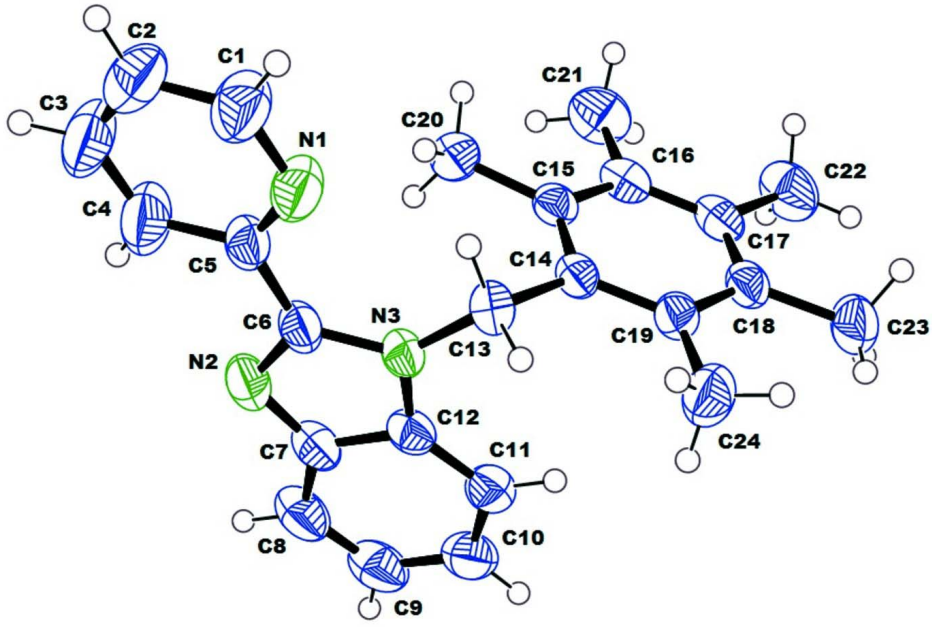


**Figure 1**

*ORTEP-3* of the title compound, showing displacement ellipsoids drawn at 50% probability level.

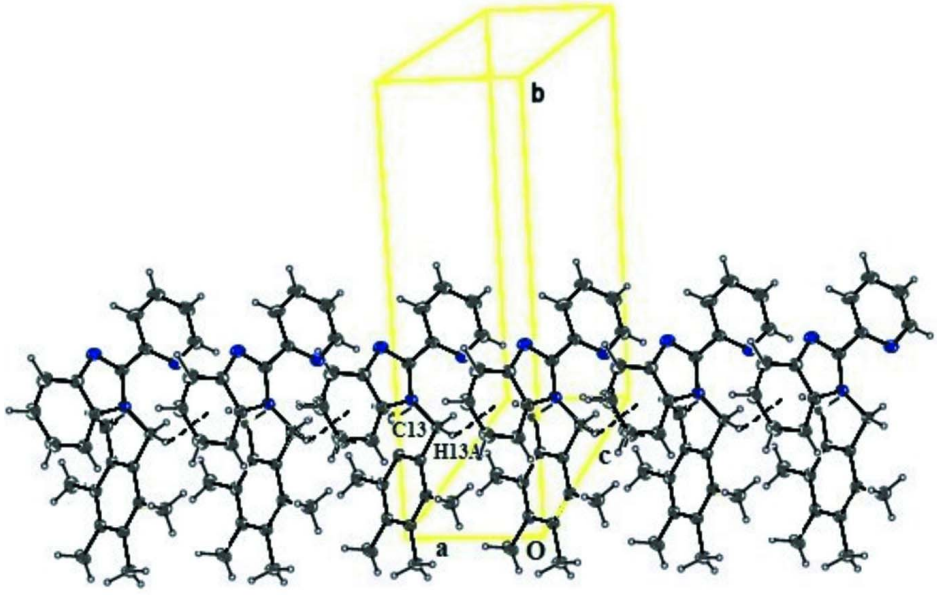


**Figure 2**

The stacking of the title compound along the *a* axis with C—H···$\pi$ type hydrogen-bond interactions (dashed lines). Displacement ellipsoids are drawn at the 50% probability level.

### 1-(2,3,4,5,6-Pentamethylbenzyl)-2-(pyridin-2-yl)-1*H*-benzimidazole

*Crystal data*

$C_{24}H_{25}N_3$
$M_r$ = 355.47

Monoclinic, $P2_1/n$
$a$ = 5.3470 (3) Å

$b$ = 21.0622 (12) Å
$c$ = 17.0379 (9) Å
$\beta$ = 97.699 (3)°
$V$ = 1901.50 (18) Å$^3$
$Z$ = 4
$F(000)$ = 760
$D_x$ = 1.242 Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1276 reflections
$\theta$ = 2.3–31.5°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 296 K
Prism, yellow
0.25 × 0.20 × 0.15 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min}$ = 0.982, $T_{max}$ = 0.989
25354 measured reflections

3741 independent reflections
3056 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.3°
$h$ = −6→6
$k$ = −25→25
$l$ = −21→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.150
$S$ = 1.04
3741 reflections
254 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.5927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

*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.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 1.0873 (5) | 0.86580 (11) | 0.44231 (14) | 0.0724 (6) |
| H1 | 1.2174 | 0.8428 | 0.4246 | 0.087* |
| C2 | 1.0060 (5) | 0.91952 (12) | 0.40152 (14) | 0.0737 (6) |
| H2 | 1.0790 | 0.9327 | 0.3577 | 0.088* |
| C3 | 0.8151 (5) | 0.95308 (12) | 0.42706 (16) | 0.0842 (7) |
| H3 | 0.7548 | 0.9900 | 0.4011 | 0.101* |
| C4 | 0.7133 (5) | 0.93151 (10) | 0.49165 (15) | 0.0771 (7) |
| H4 | 0.5809 | 0.9535 | 0.5094 | 0.092* |
| C5 | 0.8068 (3) | 0.87716 (7) | 0.53054 (11) | 0.0465 (4) |
| C6 | 0.6926 (3) | 0.85653 (7) | 0.60059 (10) | 0.0452 (4) |
| C7 | 0.4595 (4) | 0.86110 (8) | 0.69313 (11) | 0.0507 (4) |
| C8 | 0.2891 (4) | 0.87790 (10) | 0.74483 (13) | 0.0658 (6) |
| H8 | 0.2014 | 0.9161 | 0.7387 | 0.079* |

| | | | | |
|---|---|---|---|---|
| C9 | 0.2541 (4) | 0.83708 (10) | 0.80460 (13) | 0.0667 (6) |
| H9 | 0.1414 | 0.8477 | 0.8396 | 0.080* |
| C10 | 0.3850 (4) | 0.77962 (10) | 0.81392 (12) | 0.0598 (5) |
| H10 | 0.3597 | 0.7531 | 0.8558 | 0.072* |
| C11 | 0.5507 (4) | 0.76104 (9) | 0.76284 (10) | 0.0505 (4) |
| H11 | 0.6360 | 0.7225 | 0.7690 | 0.061* |
| C12 | 0.5841 (3) | 0.80251 (8) | 0.70185 (10) | 0.0432 (4) |
| C13 | 0.8894 (3) | 0.74472 (7) | 0.62583 (10) | 0.0422 (4) |
| H13A | 1.0264 | 0.7410 | 0.6691 | 0.051* |
| H13B | 0.9632 | 0.7525 | 0.5777 | 0.051* |
| C14 | 0.7459 (3) | 0.68215 (7) | 0.61734 (9) | 0.0370 (4) |
| C15 | 0.5434 (3) | 0.67529 (7) | 0.55618 (9) | 0.0391 (4) |
| C16 | 0.4047 (3) | 0.61901 (8) | 0.54888 (10) | 0.0452 (4) |
| C17 | 0.4753 (3) | 0.56796 (8) | 0.59946 (11) | 0.0471 (4) |
| C18 | 0.6838 (3) | 0.57318 (7) | 0.65801 (10) | 0.0448 (4) |
| C19 | 0.8190 (3) | 0.63066 (7) | 0.66771 (10) | 0.0412 (4) |
| C20 | 0.4783 (4) | 0.72858 (9) | 0.49769 (10) | 0.0511 (4) |
| H20A | 0.406 (3) | 0.7111 (2) | 0.4472 (7) | 0.077* |
| H20B | 0.630 (2) | 0.7521 (5) | 0.4912 (6) | 0.077* |
| H20C | 0.357 (2) | 0.7567 (5) | 0.5172 (5) | 0.077* |
| C21 | 0.1762 (4) | 0.61342 (11) | 0.48609 (14) | 0.0703 (6) |
| H21A | 0.2254 (10) | 0.5965 (8) | 0.4399 (8) | 0.105* |
| H21B | 0.106 (2) | 0.6535 (6) | 0.4754 (8) | 0.105* |
| H21C | 0.057 (2) | 0.5868 (8) | 0.5043 (5) | 0.105* |
| C22 | 0.3235 (5) | 0.50692 (10) | 0.59025 (15) | 0.0710 (6) |
| H22A | 0.314 (3) | 0.4923 (5) | 0.5373 (9) | 0.107* |
| H22B | 0.158 (3) | 0.5146 (2) | 0.6025 (10) | 0.107* |
| H22C | 0.403 (2) | 0.4757 (5) | 0.6251 (9) | 0.107* |
| C23 | 0.7616 (5) | 0.51661 (9) | 0.71064 (13) | 0.0655 (6) |
| H23A | 0.626 (2) | 0.5047 (5) | 0.7383 (8) | 0.098* |
| H23B | 0.904 (3) | 0.5276 (3) | 0.7476 (8) | 0.098* |
| H23C | 0.803 (3) | 0.4820 (6) | 0.6790 (5) | 0.098* |
| C24 | 1.0435 (4) | 0.63574 (10) | 0.73176 (13) | 0.0630 (5) |
| H24A | 1.168 (2) | 0.6592 (7) | 0.7134 (4) | 0.094* |
| H24B | 1.104 (2) | 0.5960 (6) | 0.7452 (7) | 0.094* |
| H24C | 0.9950 (10) | 0.6551 (7) | 0.7754 (7) | 0.094* |
| N1 | 0.9926 (3) | 0.84413 (8) | 0.50574 (10) | 0.0616 (4) |
| N2 | 0.5315 (3) | 0.89400 (7) | 0.63031 (10) | 0.0561 (4) |
| N3 | 0.7309 (3) | 0.79969 (6) | 0.64092 (8) | 0.0406 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0797 (15) | 0.0651 (13) | 0.0780 (14) | 0.0052 (11) | 0.0312 (12) | 0.0205 (11) |
| C2 | 0.0844 (16) | 0.0737 (14) | 0.0641 (13) | −0.0104 (12) | 0.0138 (12) | 0.0232 (11) |
| C3 | 0.1041 (19) | 0.0620 (14) | 0.0871 (17) | 0.0111 (13) | 0.0152 (15) | 0.0351 (13) |
| C4 | 0.0940 (17) | 0.0516 (12) | 0.0889 (16) | 0.0184 (11) | 0.0244 (14) | 0.0216 (11) |
| C5 | 0.0539 (10) | 0.0329 (8) | 0.0517 (10) | −0.0066 (7) | 0.0031 (8) | 0.0006 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0522 (10) | 0.0305 (8) | 0.0519 (10) | −0.0019 (7) | 0.0034 (8) | −0.0032 (7) |
| C7 | 0.0580 (11) | 0.0396 (9) | 0.0551 (10) | −0.0025 (8) | 0.0099 (9) | −0.0119 (8) |
| C8 | 0.0756 (14) | 0.0522 (11) | 0.0726 (13) | 0.0050 (10) | 0.0212 (11) | −0.0188 (10) |
| C9 | 0.0737 (14) | 0.0657 (13) | 0.0651 (13) | −0.0053 (11) | 0.0261 (11) | −0.0210 (11) |
| C10 | 0.0732 (13) | 0.0590 (11) | 0.0490 (10) | −0.0122 (10) | 0.0152 (9) | −0.0084 (9) |
| C11 | 0.0582 (11) | 0.0457 (9) | 0.0476 (10) | −0.0050 (8) | 0.0070 (8) | −0.0042 (7) |
| C12 | 0.0451 (9) | 0.0397 (8) | 0.0442 (9) | −0.0072 (7) | 0.0038 (7) | −0.0087 (7) |
| C13 | 0.0405 (9) | 0.0345 (8) | 0.0514 (9) | 0.0012 (6) | 0.0059 (7) | 0.0014 (7) |
| C14 | 0.0395 (8) | 0.0319 (7) | 0.0407 (8) | 0.0008 (6) | 0.0096 (6) | −0.0031 (6) |
| C15 | 0.0416 (8) | 0.0382 (8) | 0.0389 (8) | 0.0030 (6) | 0.0108 (7) | −0.0045 (6) |
| C16 | 0.0441 (9) | 0.0449 (9) | 0.0479 (9) | −0.0036 (7) | 0.0108 (7) | −0.0122 (7) |
| C17 | 0.0536 (10) | 0.0381 (9) | 0.0538 (10) | −0.0077 (7) | 0.0227 (8) | −0.0116 (7) |
| C18 | 0.0574 (10) | 0.0339 (8) | 0.0473 (9) | 0.0041 (7) | 0.0230 (8) | −0.0003 (7) |
| C19 | 0.0453 (9) | 0.0367 (8) | 0.0426 (8) | 0.0044 (7) | 0.0094 (7) | 0.0000 (6) |
| C20 | 0.0573 (11) | 0.0504 (10) | 0.0441 (9) | 0.0048 (8) | 0.0010 (8) | 0.0003 (8) |
| C21 | 0.0589 (12) | 0.0747 (14) | 0.0738 (14) | −0.0118 (11) | −0.0033 (11) | −0.0163 (11) |
| C22 | 0.0808 (15) | 0.0505 (11) | 0.0862 (15) | −0.0231 (10) | 0.0274 (12) | −0.0111 (10) |
| C23 | 0.0940 (16) | 0.0398 (10) | 0.0665 (13) | 0.0052 (10) | 0.0247 (11) | 0.0093 (9) |
| C24 | 0.0675 (13) | 0.0540 (11) | 0.0624 (12) | 0.0037 (9) | −0.0094 (10) | 0.0093 (9) |
| N1 | 0.0691 (10) | 0.0521 (9) | 0.0671 (10) | 0.0057 (8) | 0.0216 (8) | 0.0180 (8) |
| N2 | 0.0697 (10) | 0.0346 (7) | 0.0650 (10) | 0.0040 (7) | 0.0129 (8) | −0.0039 (7) |
| N3 | 0.0456 (7) | 0.0305 (6) | 0.0455 (7) | −0.0029 (5) | 0.0056 (6) | −0.0021 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.334 (3) | C13—H13B | 0.9700 |
| C1—C2 | 1.368 (3) | C14—C19 | 1.405 (2) |
| C1—H1 | 0.9300 | C14—C15 | 1.406 (2) |
| C2—C3 | 1.360 (4) | C15—C16 | 1.395 (2) |
| C2—H2 | 0.9300 | C15—C20 | 1.510 (2) |
| C3—C4 | 1.369 (3) | C16—C17 | 1.398 (3) |
| C3—H3 | 0.9300 | C16—C21 | 1.517 (3) |
| C4—C5 | 1.382 (3) | C17—C18 | 1.397 (3) |
| C4—H4 | 0.9300 | C17—C22 | 1.517 (2) |
| C5—N1 | 1.328 (2) | C18—C19 | 1.408 (2) |
| C5—C6 | 1.477 (3) | C18—C23 | 1.515 (2) |
| C6—N2 | 1.319 (2) | C19—C24 | 1.514 (3) |
| C6—N3 | 1.382 (2) | C20—H20A | 0.968 (12) |
| C7—N2 | 1.373 (2) | C20—H20B | 0.968 (13) |
| C7—C8 | 1.395 (3) | C20—H20C | 0.968 (12) |
| C7—C12 | 1.401 (2) | C21—H21A | 0.933 (14) |
| C8—C9 | 1.365 (3) | C21—H21B | 0.933 (14) |
| C8—H8 | 0.9300 | C21—H21C | 0.933 (14) |
| C9—C10 | 1.396 (3) | C22—H22A | 0.948 (14) |
| C9—H9 | 0.9300 | C22—H22B | 0.948 (14) |
| C10—C11 | 1.379 (3) | C22—H22C | 0.948 (14) |
| C10—H10 | 0.9300 | C23—H23A | 0.951 (14) |
| C11—C12 | 1.387 (2) | C23—H23B | 0.951 (14) |

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| C11—H11 | 0.9300 | C23—H23C | 0.951 (13) |
| C12—N3 | 1.384 (2) | C24—H24A | 0.915 (14) |
| C13—N3 | 1.478 (2) | C24—H24B | 0.915 (13) |
| C13—C14 | 1.522 (2) | C24—H24C | 0.915 (13) |
| C13—H13A | 0.9700 | | |

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| N1—C1—C2 | 124.4 (2) | C15—C16—C17 | 120.14 (16) |
| N1—C1—H1 | 117.8 | C15—C16—C21 | 119.82 (17) |
| C2—C1—H1 | 117.8 | C17—C16—C21 | 120.05 (16) |
| C3—C2—C1 | 117.9 (2) | C18—C17—C16 | 120.23 (15) |
| C3—C2—H2 | 121.0 | C18—C17—C22 | 120.34 (17) |
| C1—C2—H2 | 121.0 | C16—C17—C22 | 119.42 (18) |
| C2—C3—C4 | 118.7 (2) | C17—C18—C19 | 119.95 (15) |
| C2—C3—H3 | 120.6 | C17—C18—C23 | 119.35 (16) |
| C4—C3—H3 | 120.6 | C19—C18—C23 | 120.69 (17) |
| C3—C4—C5 | 120.2 (2) | C14—C19—C18 | 119.69 (15) |
| C3—C4—H4 | 119.9 | C14—C19—C24 | 120.95 (15) |
| C5—C4—H4 | 119.9 | C18—C19—C24 | 119.35 (15) |
| N1—C5—C4 | 121.30 (19) | C15—C20—H20A | 109.5 |
| N1—C5—C6 | 120.74 (15) | C15—C20—H20B | 109.5 |
| C4—C5—C6 | 117.96 (18) | H20A—C20—H20B | 109.5 |
| N2—C6—N3 | 112.86 (16) | C15—C20—H20C | 109.5 |
| N2—C6—C5 | 119.77 (15) | H20A—C20—H20C | 109.5 |
| N3—C6—C5 | 127.37 (15) | H20B—C20—H20C | 109.5 |
| N2—C7—C8 | 129.74 (18) | C16—C21—H21A | 109.5 |
| N2—C7—C12 | 110.39 (16) | C16—C21—H21B | 109.5 |
| C8—C7—C12 | 119.87 (18) | H21A—C21—H21B | 109.5 |
| C9—C8—C7 | 118.6 (2) | C16—C21—H21C | 109.5 |
| C9—C8—H8 | 120.7 | H21A—C21—H21C | 109.5 |
| C7—C8—H8 | 120.7 | H21B—C21—H21C | 109.5 |
| C8—C9—C10 | 120.93 (19) | C17—C22—H22A | 109.5 |
| C8—C9—H9 | 119.5 | C17—C22—H22B | 109.5 |
| C10—C9—H9 | 119.5 | H22A—C22—H22B | 109.5 |
| C11—C10—C9 | 121.92 (19) | C17—C22—H22C | 109.5 |
| C11—C10—H10 | 119.0 | H22A—C22—H22C | 109.5 |
| C9—C10—H10 | 119.0 | H22B—C22—H22C | 109.5 |
| C10—C11—C12 | 116.88 (18) | C18—C23—H23A | 109.5 |
| C10—C11—H11 | 121.6 | C18—C23—H23B | 109.5 |
| C12—C11—H11 | 121.6 | H23A—C23—H23B | 109.5 |
| N3—C12—C11 | 132.66 (16) | C18—C23—H23C | 109.5 |
| N3—C12—C7 | 105.53 (15) | H23A—C23—H23C | 109.5 |
| C11—C12—C7 | 121.80 (17) | H23B—C23—H23C | 109.5 |
| N3—C13—C14 | 113.67 (13) | C19—C24—H24A | 109.5 |
| N3—C13—H13A | 108.8 | C19—C24—H24B | 109.5 |
| C14—C13—H13A | 108.8 | H24A—C24—H24B | 109.5 |
| N3—C13—H13B | 108.8 | C19—C24—H24C | 109.5 |
| C14—C13—H13B | 108.8 | H24A—C24—H24C | 109.5 |
| H13A—C13—H13B | 107.7 | H24B—C24—H24C | 109.5 |

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| C19—C14—C15 | 119.78 (14) | C5—N1—C1 | 117.39 (17) |
| C19—C14—C13 | 120.99 (14) | C6—N2—C7 | 105.26 (15) |
| C15—C14—C13 | 119.19 (14) | C6—N3—C12 | 105.94 (13) |
| C16—C15—C14 | 120.06 (15) | C6—N3—C13 | 129.98 (14) |
| C16—C15—C20 | 119.99 (15) | C12—N3—C13 | 124.08 (13) |
| C14—C15—C20 | 119.95 (14) | | |

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| N1—C1—C2—C3 | −0.2 (4) | C15—C16—C17—C22 | −179.52 (16) |
| C1—C2—C3—C4 | −0.3 (4) | C21—C16—C17—C22 | 0.7 (3) |
| C2—C3—C4—C5 | 1.0 (4) | C16—C17—C18—C19 | 1.9 (2) |
| C3—C4—C5—N1 | −1.2 (4) | C22—C17—C18—C19 | −178.06 (16) |
| C3—C4—C5—C6 | 179.1 (2) | C16—C17—C18—C23 | −178.23 (16) |
| N1—C5—C6—N2 | 171.36 (17) | C22—C17—C18—C23 | 1.8 (2) |
| C4—C5—C6—N2 | −9.0 (3) | C15—C14—C19—C18 | −1.9 (2) |
| N1—C5—C6—N3 | −9.7 (3) | C13—C14—C19—C18 | −179.49 (14) |
| C4—C5—C6—N3 | 169.96 (19) | C15—C14—C19—C24 | 177.28 (16) |
| N2—C7—C8—C9 | −178.4 (2) | C13—C14—C19—C24 | −0.3 (2) |
| C12—C7—C8—C9 | 1.9 (3) | C17—C18—C19—C14 | −1.2 (2) |
| C7—C8—C9—C10 | −0.1 (3) | C23—C18—C19—C14 | 178.93 (15) |
| C8—C9—C10—C11 | −1.2 (3) | C17—C18—C19—C24 | 179.62 (16) |
| C9—C10—C11—C12 | 0.7 (3) | C23—C18—C19—C24 | −0.3 (2) |
| C10—C11—C12—N3 | −179.82 (17) | C4—C5—N1—C1 | 0.7 (3) |
| C10—C11—C12—C7 | 1.1 (3) | C6—C5—N1—C1 | −179.67 (18) |
| N2—C7—C12—N3 | −1.48 (19) | C2—C1—N1—C5 | 0.1 (4) |
| C8—C7—C12—N3 | 178.23 (17) | N3—C6—N2—C7 | 0.2 (2) |
| N2—C7—C12—C11 | 177.79 (16) | C5—C6—N2—C7 | 179.26 (15) |
| C8—C7—C12—C11 | −2.5 (3) | C8—C7—N2—C6 | −178.8 (2) |
| N3—C13—C14—C19 | −121.53 (16) | C12—C7—N2—C6 | 0.8 (2) |
| N3—C13—C14—C15 | 60.88 (19) | N2—C6—N3—C12 | −1.10 (19) |
| C19—C14—C15—C16 | 4.3 (2) | C5—C6—N3—C12 | 179.91 (16) |
| C13—C14—C15—C16 | −178.05 (14) | N2—C6—N3—C13 | 178.34 (15) |
| C19—C14—C15—C20 | −174.84 (15) | C5—C6—N3—C13 | −0.7 (3) |
| C13—C14—C15—C20 | 2.8 (2) | C11—C12—N3—C6 | −177.65 (18) |
| C14—C15—C16—C17 | −3.6 (2) | C7—C12—N3—C6 | 1.50 (17) |
| C20—C15—C16—C17 | 175.52 (15) | C11—C12—N3—C13 | 2.9 (3) |
| C14—C15—C16—C21 | 176.10 (16) | C7—C12—N3—C13 | −177.98 (14) |
| C20—C15—C16—C21 | −4.7 (2) | C14—C13—N3—C6 | −125.33 (17) |
| C15—C16—C17—C18 | 0.5 (2) | C14—C13—N3—C12 | 54.0 (2) |
| C21—C16—C17—C18 | −179.21 (16) | | |

*Hydrogen-bond geometry (Å, º)*

Cg is the centroid of the C7–C12 benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13*A*···*Cg*$^{i}$ | 0.97 | 2.91 | 3.6941 (18) | 139 |
| C13—H13*B*···N1 | 0.97 | 2.30 | 3.029 (2) | 131 |

Symmetry code: (i) *x*−1, *y*, *z*.