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# 2-Methyl-3-*p*-tolyl-3*H*-benzo[e]indole-1-carbonitrile

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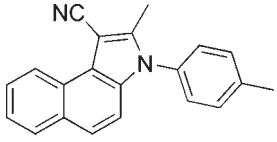
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.056; $wR$ factor = 0.168; data-to-parameter ratio = 13.6.

In the title compound, $C_{21}H_{16}N_2$, the dihedral angle between the benzoindole and tosyl ring systems is 71.99 (7)°. In the crystal, molecules are linked into centrosymmetric dimers by pairs of C—H···N hydrogen bonds, generating $R_2^2(16)$ loops.

## Related literature

For the synthesis, see: Du *et al.* (2006).




## Experimental

### Crystal data

$C_{21}H_{16}N_2$
$M_r$ = 296.36
Monoclinic, $P2_1/n$
$a$ = 10.321 (2) Å
$b$ = 12.422 (3) Å
$c$ = 13.258 (3) Å
$\beta$ = 107.14 (3)°
$V$ = 1624.4 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 293 K
0.28 × 0.20 × 0.18 mm

### Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.980, $T_{max}$ = 0.987
10714 measured reflections
2858 independent reflections
2092 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.168
$S$ = 1.04
2858 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C16—H16···N2$^{i}$ | 0.93 | 2.60 | 3.480 (3) | 158 |

Symmetry code: (i) $-x, -y+2, -z$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5275).

## References

Du, Y. F., Liu, R. H., Linn, G. & Zhao, K. (2006). *Org. Lett.* **8**, 5919–5922.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2010). E**66**, o111 [doi:10.1107/S1600536809052441]

## 2-Methyl-3-*p*-tolyl-3*H*-benzo[e]indole-1-carbonitrile

**Jiang-Sheng Li, Qi-Xi He and Peng-Yu Li**

### S1. Comment

The title compound, (I), comprises of a benzoindole ring and tosyl ring (Fig. 1). The dihedral angle of both rings is 71.99 (7)°.

In the crystal packing, molecules are linked into centrosymmetric dimers by C—H···N hydrogen bonds (Table 1). Weak C—H···$\pi$ interactions help dimers pack. No significant $\pi$-$\pi$ stacking interaction was observed.

### S2. Experimental

The compound was obtained according to the method of Du and his coworkers (2006). Colourless block of (I) was grown by slow evaporation of its ethanolic solution.

### S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å)and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(CH) or 1.5$U_{eq}$($CH_3$).

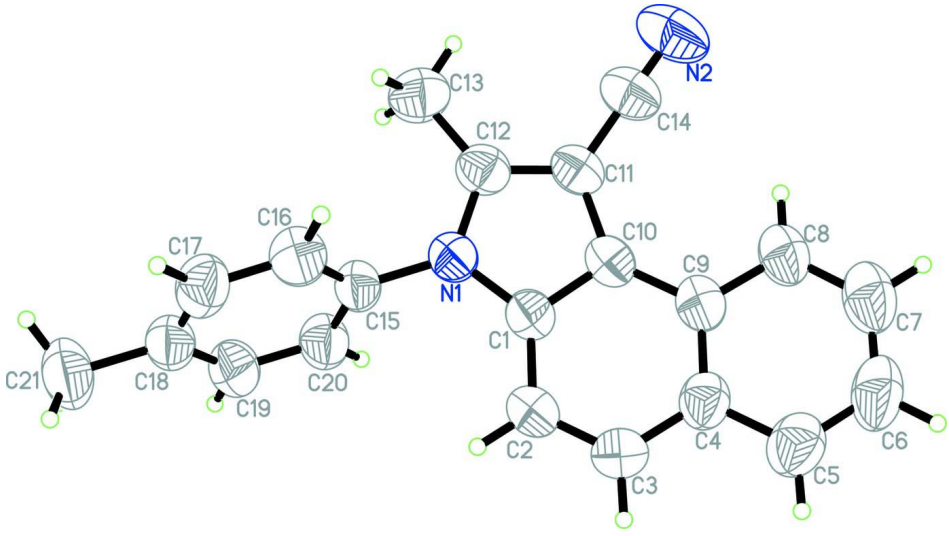



**Figure 1**

The molecule of (I) showing displacement ellipsoids drawn at the 50% probability level.

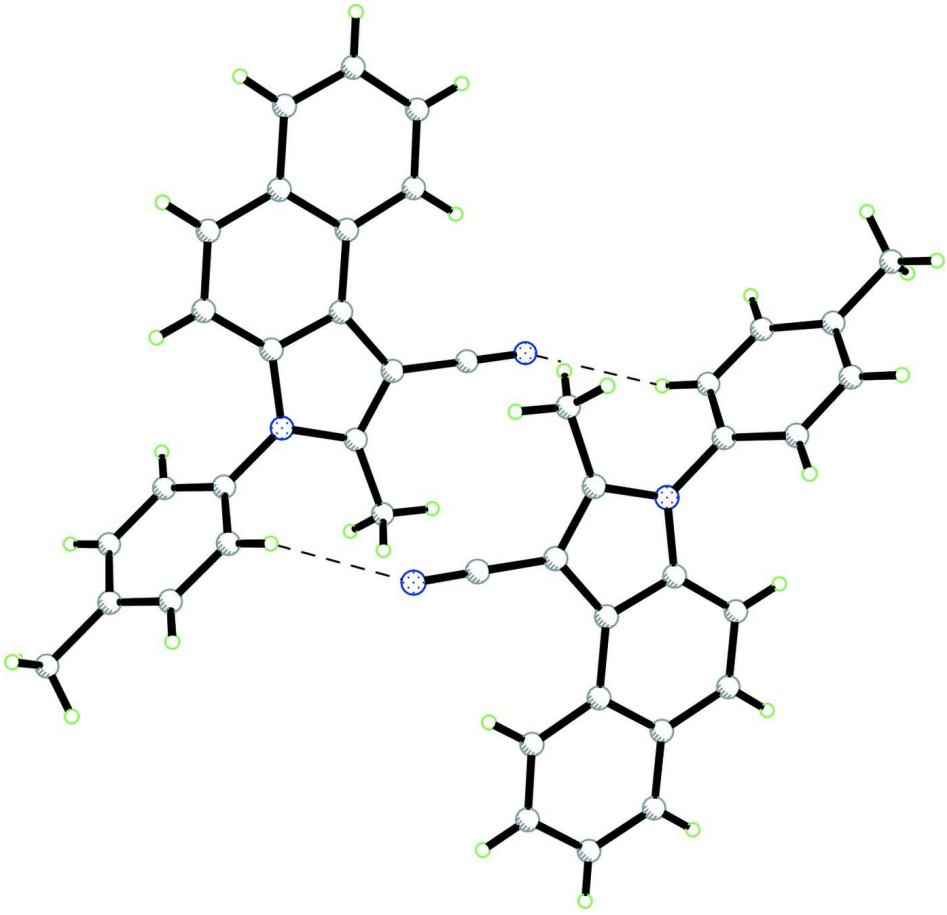


**Figure 2**

Centrosymmetric dimers of (I) formed by C—H···N hydrogen bonds drawn as dashed lines.

### 2-Methyl-3-*p*-tolyl-3*H*-benzo[*e*]indole-1-carbonitrile

*Crystal data*

$C_{21}H_{16}N_2$
$M_r = 296.36$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.321$ (2) Å
$b = 12.422$ (3) Å
$c = 13.258$ (3) Å
$\beta = 107.14$ (3)°
$V = 1624.4$ (6) Å$^3$
$Z = 4$
$F(000) = 624$
$D_x = 1.212$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3474 reflections
$\theta = 2.2$–27.5°
$\mu = 0.07$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.28 × 0.20 × 0.18 mm

*Data collection*

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.980$, $T_{max} = 0.987$
10714 measured reflections
2858 independent reflections
2092 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$

$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.2°
$h$ = −12→11
$k$ = −13→14
$l$ = −15→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.168
$S$ = 1.04
2858 reflections
210 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
$w = 1/[\sigma^2(F_o^2) + (0.1027P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.070 (10)

*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 based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.10089 (15) | 0.87702 (12) | 0.23973 (11) | 0.0575 (5) |
| N2 | −0.2675 (2) | 1.06928 (18) | 0.01735 (16) | 0.1025 (8) |
| C1 | 0.00439 (18) | 0.79674 (14) | 0.23281 (13) | 0.0547 (5) |
| C2 | 0.0217 (2) | 0.69469 (15) | 0.27979 (14) | 0.0629 (5) |
| H2 | 0.1053 | 0.6728 | 0.3241 | 0.075* |
| C3 | −0.0883 (2) | 0.62878 (16) | 0.25826 (15) | 0.0679 (6) |
| H3 | −0.0790 | 0.5606 | 0.2885 | 0.081* |
| C4 | −0.2171 (2) | 0.66084 (17) | 0.19091 (15) | 0.0631 (6) |
| C5 | −0.3298 (2) | 0.5901 (2) | 0.16630 (16) | 0.0806 (7) |
| H5 | −0.3197 | 0.5211 | 0.1947 | 0.097* |
| C6 | −0.4540 (2) | 0.6220 (2) | 0.10095 (19) | 0.0900 (8) |
| H6 | −0.5266 | 0.5742 | 0.0854 | 0.108* |
| C7 | −0.4715 (2) | 0.7253 (2) | 0.05799 (18) | 0.0860 (7) |
| H7 | −0.5561 | 0.7467 | 0.0150 | 0.103* |
| C8 | −0.3656 (2) | 0.79452 (19) | 0.07884 (15) | 0.0692 (6) |
| H8 | −0.3783 | 0.8630 | 0.0491 | 0.083* |
| C9 | −0.23647 (19) | 0.76498 (16) | 0.14464 (13) | 0.0580 (5) |
| C10 | −0.12000 (19) | 0.83318 (14) | 0.16682 (12) | 0.0542 (5) |
| C11 | −0.0941 (2) | 0.93897 (14) | 0.13370 (13) | 0.0589 (5) |
| C12 | 0.0402 (2) | 0.96343 (15) | 0.17945 (14) | 0.0608 (5) |
| C13 | 0.1146 (3) | 1.06418 (17) | 0.17368 (17) | 0.0812 (7) |

| | | | | |
|---|---|---|---|---|
| H13A | 0.1546 | 1.0918 | 0.2436 | 0.122* |
| H13B | 0.0529 | 1.1164 | 0.1323 | 0.122* |
| H13C | 0.1847 | 1.0496 | 0.1414 | 0.122* |
| C14 | −0.1898 (2) | 1.01126 (18) | 0.06895 (15) | 0.0722 (6) |
| C15 | 0.24140 (19) | 0.86902 (14) | 0.29878 (14) | 0.0556 (5) |
| C16 | 0.3392 (2) | 0.85881 (17) | 0.24716 (15) | 0.0670 (6) |
| H16 | 0.3146 | 0.8569 | 0.1738 | 0.080* |
| C17 | 0.4734 (2) | 0.85143 (16) | 0.30554 (17) | 0.0722 (6) |
| H17 | 0.5388 | 0.8442 | 0.2704 | 0.087* |
| C18 | 0.5142 (2) | 0.85442 (15) | 0.41425 (17) | 0.0670 (6) |
| C19 | 0.4147 (2) | 0.86356 (17) | 0.46373 (16) | 0.0717 (6) |
| H19 | 0.4395 | 0.8647 | 0.5371 | 0.086* |
| C20 | 0.2793 (2) | 0.87108 (16) | 0.40767 (14) | 0.0661 (6) |
| H20 | 0.2140 | 0.8775 | 0.4430 | 0.079* |
| C21 | 0.6620 (2) | 0.8465 (2) | 0.4766 (2) | 0.1000 (9) |
| H21A | 0.6952 | 0.7759 | 0.4682 | 0.150* |
| H21B | 0.6720 | 0.8594 | 0.5499 | 0.150* |
| H21C | 0.7128 | 0.8993 | 0.4513 | 0.150* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0540 (10) | 0.0542 (9) | 0.0598 (9) | 0.0010 (7) | 0.0098 (7) | 0.0032 (7) |
| N2 | 0.1048 (18) | 0.1026 (16) | 0.0931 (13) | 0.0401 (13) | 0.0185 (12) | 0.0307 (12) |
| C1 | 0.0532 (11) | 0.0564 (11) | 0.0521 (9) | 0.0020 (9) | 0.0115 (8) | 0.0003 (8) |
| C2 | 0.0582 (12) | 0.0630 (12) | 0.0618 (11) | 0.0065 (10) | 0.0091 (9) | 0.0085 (9) |
| C3 | 0.0706 (15) | 0.0630 (12) | 0.0686 (12) | −0.0020 (10) | 0.0181 (10) | 0.0123 (9) |
| C4 | 0.0561 (13) | 0.0752 (14) | 0.0595 (11) | −0.0083 (10) | 0.0193 (9) | −0.0022 (9) |
| C5 | 0.0756 (17) | 0.0909 (16) | 0.0801 (13) | −0.0151 (13) | 0.0306 (12) | −0.0002 (11) |
| C6 | 0.0581 (16) | 0.124 (2) | 0.0903 (16) | −0.0246 (14) | 0.0249 (13) | −0.0114 (15) |
| C7 | 0.0544 (14) | 0.123 (2) | 0.0797 (14) | −0.0008 (13) | 0.0185 (11) | −0.0047 (14) |
| C8 | 0.0516 (12) | 0.0883 (15) | 0.0654 (12) | 0.0054 (11) | 0.0137 (9) | −0.0024 (10) |
| C9 | 0.0517 (12) | 0.0728 (13) | 0.0502 (10) | 0.0031 (9) | 0.0162 (8) | −0.0029 (8) |
| C10 | 0.0531 (11) | 0.0601 (11) | 0.0475 (9) | 0.0074 (9) | 0.0120 (8) | −0.0010 (7) |
| C11 | 0.0616 (13) | 0.0571 (11) | 0.0550 (10) | 0.0116 (9) | 0.0128 (9) | 0.0036 (8) |
| C12 | 0.0653 (13) | 0.0532 (11) | 0.0628 (10) | 0.0061 (9) | 0.0171 (9) | 0.0013 (8) |
| C13 | 0.0884 (17) | 0.0583 (13) | 0.0960 (14) | −0.0013 (11) | 0.0257 (13) | 0.0075 (11) |
| C14 | 0.0755 (15) | 0.0725 (14) | 0.0667 (12) | 0.0194 (11) | 0.0181 (10) | 0.0103 (10) |
| C15 | 0.0481 (11) | 0.0550 (11) | 0.0584 (10) | −0.0029 (8) | 0.0078 (8) | −0.0001 (8) |
| C16 | 0.0665 (14) | 0.0746 (13) | 0.0614 (11) | 0.0013 (10) | 0.0213 (10) | −0.0024 (9) |
| C17 | 0.0578 (14) | 0.0732 (14) | 0.0902 (15) | 0.0001 (10) | 0.0288 (11) | −0.0033 (10) |
| C18 | 0.0535 (13) | 0.0555 (12) | 0.0852 (14) | −0.0010 (9) | 0.0102 (11) | 0.0016 (10) |
| C19 | 0.0628 (14) | 0.0818 (14) | 0.0627 (11) | −0.0043 (11) | 0.0062 (10) | 0.0005 (10) |
| C20 | 0.0564 (13) | 0.0825 (14) | 0.0593 (11) | −0.0021 (10) | 0.0169 (9) | 0.0014 (9) |
| C21 | 0.0563 (15) | 0.0937 (18) | 0.133 (2) | 0.0003 (12) | 0.0011 (14) | 0.0023 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C12 | 1.374 (2) | C10—C11 | 1.435 (3) |
| N1—C1 | 1.393 (2) | C11—C12 | 1.373 (3) |
| N1—C15 | 1.434 (2) | C11—C14 | 1.421 (3) |
| N2—C14 | 1.143 (2) | C12—C13 | 1.483 (3) |
| C1—C10 | 1.399 (2) | C13—H13A | 0.9600 |
| C1—C2 | 1.400 (2) | C13—H13B | 0.9600 |
| C2—C3 | 1.360 (3) | C13—H13C | 0.9600 |
| C2—H2 | 0.9300 | C15—C20 | 1.380 (3) |
| C3—C4 | 1.422 (3) | C15—C16 | 1.382 (3) |
| C3—H3 | 0.9300 | C16—C17 | 1.376 (3) |
| C4—C5 | 1.417 (3) | C16—H16 | 0.9300 |
| C4—C9 | 1.420 (3) | C17—C18 | 1.378 (3) |
| C5—C6 | 1.377 (3) | C17—H17 | 0.9300 |
| C5—H5 | 0.9300 | C18—C19 | 1.376 (3) |
| C6—C7 | 1.394 (4) | C18—C21 | 1.509 (3) |
| C6—H6 | 0.9300 | C19—C20 | 1.379 (3) |
| C7—C8 | 1.354 (3) | C19—H19 | 0.9300 |
| C7—H7 | 0.9300 | C20—H20 | 0.9300 |
| C8—C9 | 1.409 (3) | C21—H21A | 0.9600 |
| C8—H8 | 0.9300 | C21—H21B | 0.9600 |
| C9—C10 | 1.429 (3) | C21—H21C | 0.9600 |
| | | | |
| C12—N1—C1 | 109.04 (15) | C14—C11—C10 | 127.20 (19) |
| C12—N1—C15 | 125.88 (15) | C11—C12—N1 | 108.18 (17) |
| C1—N1—C15 | 125.07 (14) | C11—C12—C13 | 129.44 (18) |
| N1—C1—C10 | 108.42 (15) | N1—C12—C13 | 122.34 (18) |
| N1—C1—C2 | 128.59 (17) | C12—C13—H13A | 109.5 |
| C10—C1—C2 | 122.97 (17) | C12—C13—H13B | 109.5 |
| C3—C2—C1 | 117.55 (18) | H13A—C13—H13B | 109.5 |
| C3—C2—H2 | 121.2 | C12—C13—H13C | 109.5 |
| C1—C2—H2 | 121.2 | H13A—C13—H13C | 109.5 |
| C2—C3—C4 | 122.07 (18) | H13B—C13—H13C | 109.5 |
| C2—C3—H3 | 119.0 | N2—C14—C11 | 179.4 (3) |
| C4—C3—H3 | 119.0 | C20—C15—C16 | 119.78 (18) |
| C5—C4—C9 | 117.6 (2) | C20—C15—N1 | 119.91 (18) |
| C5—C4—C3 | 121.5 (2) | C16—C15—N1 | 120.31 (16) |
| C9—C4—C3 | 120.85 (18) | C17—C16—C15 | 119.24 (17) |
| C6—C5—C4 | 121.0 (2) | C17—C16—H16 | 120.4 |
| C6—C5—H5 | 119.5 | C15—C16—H16 | 120.4 |
| C4—C5—H5 | 119.5 | C16—C17—C18 | 122.2 (2) |
| C5—C6—C7 | 120.4 (2) | C16—C17—H17 | 118.9 |
| C5—C6—H6 | 119.8 | C18—C17—H17 | 118.9 |
| C7—C6—H6 | 119.8 | C19—C18—C17 | 117.41 (19) |
| C8—C7—C6 | 120.1 (2) | C19—C18—C21 | 121.3 (2) |
| C8—C7—H7 | 120.0 | C17—C18—C21 | 121.2 (2) |
| C6—C7—H7 | 120.0 | C18—C19—C20 | 121.91 (19) |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 121.4 (2) | C18—C19—H19 | 119.0 |
| C7—C8—H8 | 119.3 | C20—C19—H19 | 119.0 |
| C9—C8—H8 | 119.3 | C19—C20—C15 | 119.5 (2) |
| C8—C9—C4 | 119.45 (19) | C19—C20—H20 | 120.3 |
| C8—C9—C10 | 123.90 (19) | C15—C20—H20 | 120.3 |
| C4—C9—C10 | 116.63 (17) | C18—C21—H21A | 109.5 |
| C1—C10—C9 | 119.89 (17) | C18—C21—H21B | 109.4 |
| C1—C10—C11 | 105.56 (17) | H21A—C21—H21B | 109.5 |
| C9—C10—C11 | 134.53 (16) | C18—C21—H21C | 109.4 |
| C12—C11—C14 | 123.93 (19) | H21A—C21—H21C | 109.5 |
| C12—C11—C10 | 108.80 (15) | H21B—C21—H21C | 109.5 |

| | | | |
|---|---|---|---|
| C12—N1—C1—C10 | −0.03 (19) | C1—C10—C11—C12 | −0.5 (2) |
| C15—N1—C1—C10 | −178.86 (14) | C9—C10—C11—C12 | −178.67 (19) |
| C12—N1—C1—C2 | 178.88 (18) | C1—C10—C11—C14 | −177.42 (17) |
| C15—N1—C1—C2 | 0.0 (3) | C9—C10—C11—C14 | 4.4 (3) |
| N1—C1—C2—C3 | −177.95 (18) | C14—C11—C12—N1 | 177.53 (16) |
| C10—C1—C2—C3 | 0.8 (3) | C10—C11—C12—N1 | 0.5 (2) |
| C1—C2—C3—C4 | −0.1 (3) | C14—C11—C12—C13 | 0.0 (3) |
| C2—C3—C4—C5 | 177.9 (2) | C10—C11—C12—C13 | −177.0 (2) |
| C2—C3—C4—C9 | −1.2 (3) | C1—N1—C12—C11 | −0.3 (2) |
| C9—C4—C5—C6 | −0.8 (3) | C15—N1—C12—C11 | 178.55 (16) |
| C3—C4—C5—C6 | −179.95 (19) | C1—N1—C12—C13 | 177.43 (18) |
| C4—C5—C6—C7 | −0.4 (4) | C15—N1—C12—C13 | −3.8 (3) |
| C5—C6—C7—C8 | 1.2 (4) | C12—C11—C14—N2 | −129 (29) |
| C6—C7—C8—C9 | −0.7 (3) | C10—C11—C14—N2 | 47 (29) |
| C7—C8—C9—C4 | −0.6 (3) | C12—N1—C15—C20 | 110.1 (2) |
| C7—C8—C9—C10 | 177.95 (18) | C1—N1—C15—C20 | −71.3 (2) |
| C5—C4—C9—C8 | 1.3 (3) | C12—N1—C15—C16 | −70.1 (2) |
| C3—C4—C9—C8 | −179.57 (17) | C1—N1—C15—C16 | 108.5 (2) |
| C5—C4—C9—C10 | −177.31 (17) | C20—C15—C16—C17 | −0.4 (3) |
| C3—C4—C9—C10 | 1.8 (3) | N1—C15—C16—C17 | 179.90 (17) |
| N1—C1—C10—C9 | 178.82 (15) | C15—C16—C17—C18 | −0.3 (3) |
| C2—C1—C10—C9 | −0.2 (3) | C16—C17—C18—C19 | 1.0 (3) |
| N1—C1—C10—C11 | 0.30 (19) | C16—C17—C18—C21 | −179.8 (2) |
| C2—C1—C10—C11 | −178.68 (16) | C17—C18—C19—C20 | −0.9 (3) |
| C8—C9—C10—C1 | −179.70 (15) | C21—C18—C19—C20 | 179.9 (2) |
| C4—C9—C10—C1 | −1.1 (2) | C18—C19—C20—C15 | 0.3 (3) |
| C8—C9—C10—C11 | −1.7 (3) | C16—C15—C20—C19 | 0.4 (3) |
| C4—C9—C10—C11 | 176.86 (18) | N1—C15—C20—C19 | −179.86 (17) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16···N2$^{i}$ | 0.93 | 2.60 | 3.480 (3) | 158 |

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