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# 4-(5-Phenyl-1,2,4-triazolo[3,4-*a*]-isoquinolin-3-yl)benzonitrile

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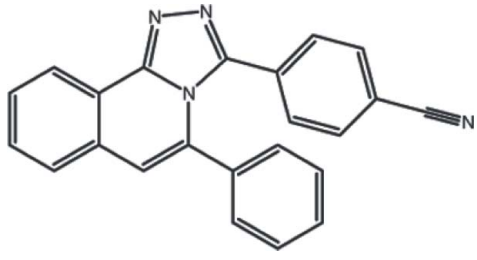
Key indicators: single-crystal X-ray study; $T$ = 290 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.046; $wR$ factor = 0.100; data-to-parameter ratio = 13.0.

In the title molecule, $C_{23}H_{14}N_4$, the triazoloisoquinoline ring system is nearly planar, with an r.m.s. deviation of 0.038 (2) Å and a maximum deviation of −0.030 (2) Å from the mean plane of the triazole ring C atom which is bonded to the benzene ring. The benzene and phenyl rings are twisted by 57.65 (8) and 53.60 (9)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. In the crystal structure, molecules are linked by weak aromatic $\pi$–$\pi$ interactions [centroid–centroid distance = 3.8074 (12) Å]. In addition, the crystal structure exhibits a nonclassical intermolecular C—H···N hydrogen bond.

## Related literature

For a related crystal structure, see: Khan *et al.* (2010).



## Experimental

### Crystal data

$C_{23}H_{14}N_4$
$M_r$ = 346.38
Orthorhombic, *Pbca*
$a$ = 7.1614 (3) Å
$b$ = 18.0957 (7) Å
$c$ = 26.4021 (9) Å
$V$ = 3421.5 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 290 K
0.25 × 0.21 × 0.17 mm

### Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.959, $T_{max}$ = 0.986
14977 measured reflections
3164 independent reflections
1490 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.070

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.100
$S$ = 0.81
3164 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C11—H11···N3$^{i}$ | 0.93 | 2.50 | 3.418 (3) | 170 |

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the FIST program for data collection on the Oxford single-crystal diffractometer at SSCU, IISc, Bangalore. The authors also thank Professor T. N. Guru Row, IISc, Bangalore, for his help with the data collection. FNK thanks the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2199).

## References

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# supporting information

*Acta Cryst.* (2010). E**66**, o1081 [https://doi.org/10.1107/S1600536810013012]

## 4-(5-Phenyl-1,2,4-triazolo[3,4-*a*]isoquinolin-3-yl)benzonitrile

**F. Nawaz Khan, P. Manivel, K. Prabakaran, Venkatesha R. Hathwar and Mehmet Akkurt**

### S1. Comment

As part of our search for new isoquinoline analogues (Khan *et al.*, 2010), we focused on synthesis of titled compounds and the crystal structure is reported.

In the title molecule, Fig. 1, the triazoloisoquinoline ring system (N1-N3/C1-C9/C16) is nearly planar, with an r.m.s. deviation of 0.038 (2)Å and a maximum deviation of -0.030 (2)Å from the mean plane for the triazole ring C16 atom which is bonded to the benzene ring (C17-C22). The benzene (C17-C22) and phenyl (C10-C15) rings are twisted by 57.65 (8)° and 53.60 (9)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. The benzene (C17-C22) and phenyl (C10-C15) rings make a dihedral angle of 29.10 (11)° with each other.

Molecular conformation is stabilized by a weak $\pi$–$\pi$ interaction [Cg4···Cg5 = 3.8229 (14)Å, where are Cg4 and Cg5 are centroids of the C10-C15 and C17-C22 rings, respectively]. In the crystal structure, the molecules are linked by weak aromatic $\pi$–$\pi$ interactions [Cg1···Cg1$^{ii}$ = 3.8074 (12)Å, symmetry code: (ii) *x*-1/2, 1/2-*y*, -*z*. Cg1 is the centroid of the N1-N3/C1/C16 ring]. In addition, the crystal structure exhibits an intermolecular non-classical C–H···N hydrogen bond (Table 1, Fig. 2).

### S2. Experimental

2-(3-Phenylisoquinolin-1-yl)hydrazine (1 mmol) was condensed with 4-formylbenzonitrile (1.1 mmol) under refluxing conditions isopropanol (10 ml) solvent to give the corresponding hydrazone in high yield. After removal of solvent the compound was then oxidatively cyclized in nitrobenzene (10 ml) at 473 K. The product was recrystallized from dichloromethane to give block-shaped crystals.

### S3. Refinement

All H atoms were placed in calculated positions with C–H = 0.93Å and were included in the refinement in the riding model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

Pure diffraction experiment (ratio observed/unique reflections 47%) we explain by weak diffraction of the crystal.

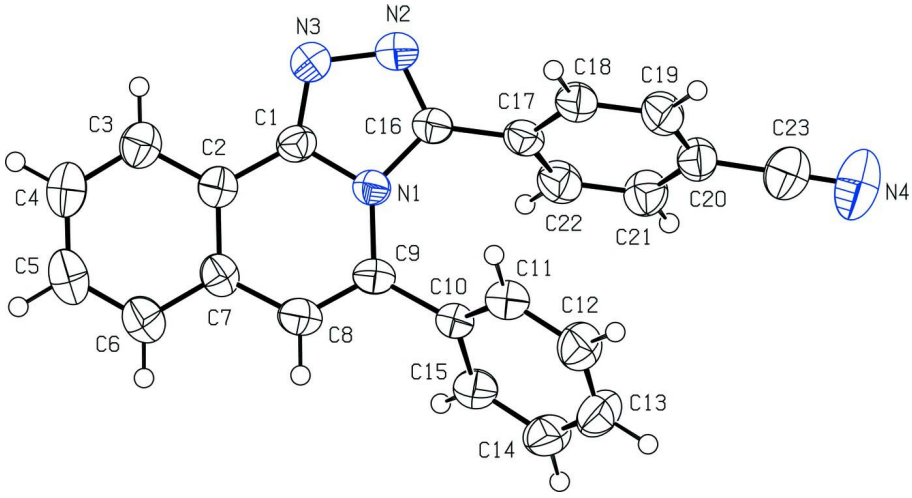


**Figure 1**

The view of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

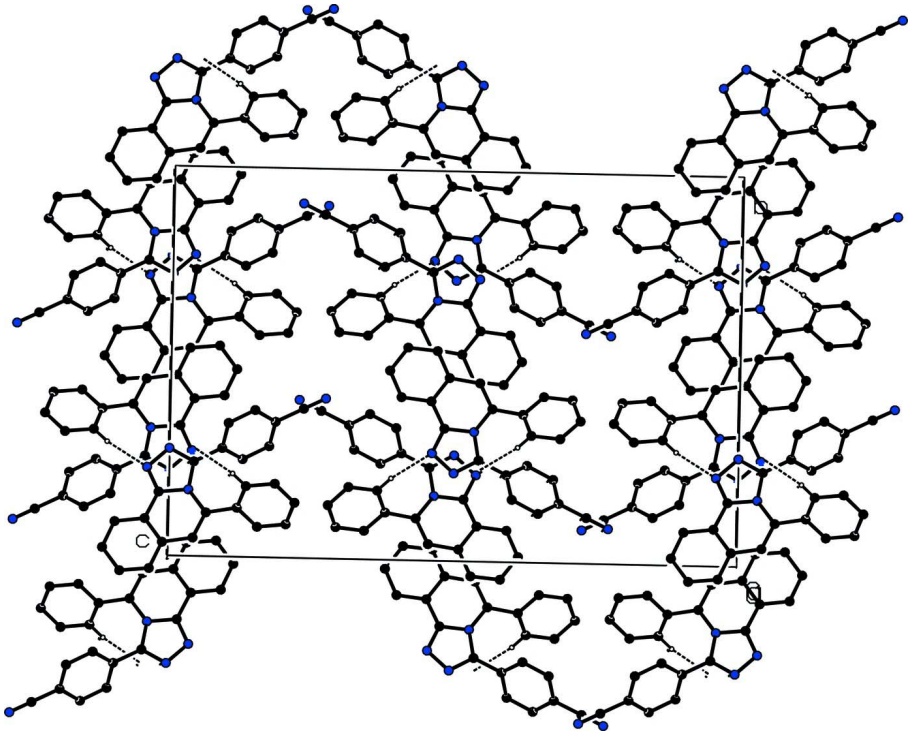

**Figure 2**

The packing diagram and the hydrogen bonding in the title crystal structure viewed down the [1 0 0] direction. H atoms not involved in the motif shown have been omitted for clarity.

**(I)**

*Crystal data*

$C_{23}H_{14}N_4$
$M_r = 346.38$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 7.1614$ (3) Å
$b = 18.0957$ (7) Å
$c = 26.4021$ (9) Å
$V = 3421.5$ (2) Å$^3$
$Z = 8$
$F(000) = 1440$
$D_x = 1.345$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1235 reflections
$\theta = 1.6$–$20.4°$
$\mu = 0.08$ mm$^{-1}$
$T = 290$ K
Block, colourless
0.25 × 0.21 × 0.17 mm

*Data collection*

Oxford Xcalibur Eos (Nova) CCD detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2009)
$T_{min} = 0.959$, $T_{max} = 0.986$
14977 measured reflections
3164 independent reflections
1490 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 7$
$k = -21 \rightarrow 21$
$l = -31 \rightarrow 31$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.100$
$S = 0.81$
3164 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 | 0.6627 (2) | 0.33099 (9) | 0.03366 (6) | 0.0370 (4) |
| N2 | 0.5820 (3) | 0.22467 (10) | −0.00072 (7) | 0.0510 (5) |
| N3 | 0.6063 (2) | 0.27481 (11) | −0.03950 (7) | 0.0495 (5) |
| N4 | 0.5390 (3) | 0.08980 (15) | 0.27259 (9) | 0.0927 (9) |
| C1 | 0.6539 (3) | 0.33812 (13) | −0.01851 (8) | 0.0395 (5) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.6915 (3) | 0.40722 (12) | −0.04237 (8) | 0.0407 (6) |
| C3 | 0.6888 (3) | 0.41638 (14) | −0.09495 (8) | 0.0490 (6) |
| H3 | 0.6586 | 0.3766 | −0.1157 | 0.059* |
| C4 | 0.7302 (3) | 0.48368 (15) | −0.11611 (9) | 0.0570 (7) |
| H4 | 0.7297 | 0.4894 | −0.1511 | 0.068* |
| C5 | 0.7728 (3) | 0.54308 (14) | −0.08507 (9) | 0.0581 (7) |
| H5 | 0.8002 | 0.5887 | −0.0996 | 0.070* |
| C6 | 0.7754 (3) | 0.53585 (13) | −0.03328 (9) | 0.0526 (6) |
| H6 | 0.8030 | 0.5764 | −0.0130 | 0.063* |
| C7 | 0.7364 (3) | 0.46741 (12) | −0.01110 (8) | 0.0416 (6) |
| C8 | 0.7527 (3) | 0.45523 (12) | 0.04249 (8) | 0.0454 (6) |
| H8 | 0.7853 | 0.4952 | 0.0628 | 0.054* |
| C9 | 0.7238 (3) | 0.38972 (12) | 0.06498 (8) | 0.0387 (6) |
| C10 | 0.7671 (3) | 0.37673 (11) | 0.11909 (8) | 0.0374 (5) |
| C11 | 0.8907 (3) | 0.32192 (12) | 0.13406 (8) | 0.0456 (6) |
| H11 | 0.9426 | 0.2903 | 0.1101 | 0.055* |
| C12 | 0.9365 (3) | 0.31454 (14) | 0.18466 (9) | 0.0562 (7) |
| H12 | 1.0180 | 0.2774 | 0.1948 | 0.067* |
| C13 | 0.8625 (4) | 0.36161 (15) | 0.22007 (9) | 0.0645 (8) |
| H13 | 0.8935 | 0.3561 | 0.2541 | 0.077* |
| C14 | 0.7438 (4) | 0.41647 (15) | 0.20553 (9) | 0.0595 (7) |
| H14 | 0.6960 | 0.4490 | 0.2295 | 0.071* |
| C15 | 0.6944 (3) | 0.42380 (13) | 0.15537 (9) | 0.0478 (6) |
| H15 | 0.6114 | 0.4608 | 0.1458 | 0.057* |
| C16 | 0.6137 (3) | 0.25837 (12) | 0.04252 (8) | 0.0406 (6) |
| C17 | 0.5906 (3) | 0.22246 (12) | 0.09194 (8) | 0.0403 (5) |
| C18 | 0.6918 (3) | 0.15870 (13) | 0.10218 (8) | 0.0480 (6) |
| H18 | 0.7701 | 0.1391 | 0.0775 | 0.058* |
| C19 | 0.6771 (3) | 0.12414 (12) | 0.14857 (9) | 0.0523 (6) |
| H19 | 0.7474 | 0.0821 | 0.1554 | 0.063* |
| C20 | 0.5575 (3) | 0.15217 (13) | 0.18497 (8) | 0.0480 (6) |
| C21 | 0.4514 (3) | 0.21414 (13) | 0.17476 (8) | 0.0524 (6) |
| H21 | 0.3693 | 0.2324 | 0.1990 | 0.063* |
| C22 | 0.4678 (3) | 0.24882 (13) | 0.12834 (8) | 0.0503 (6) |
| H22 | 0.3957 | 0.2903 | 0.1214 | 0.060* |
| C23 | 0.5459 (3) | 0.11720 (15) | 0.23405 (10) | 0.0629 (8) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0393 (10) | 0.0337 (11) | 0.0381 (11) | −0.0026 (8) | −0.0031 (8) | −0.0012 (9) |
| N2 | 0.0631 (13) | 0.0439 (12) | 0.0459 (12) | −0.0068 (10) | −0.0062 (10) | −0.0041 (11) |
| N3 | 0.0614 (13) | 0.0457 (13) | 0.0414 (11) | −0.0057 (10) | −0.0054 (9) | 0.0003 (10) |
| N4 | 0.0964 (19) | 0.124 (2) | 0.0576 (16) | 0.0151 (16) | 0.0099 (14) | 0.0261 (16) |
| C1 | 0.0394 (14) | 0.0404 (15) | 0.0387 (13) | −0.0003 (11) | −0.0054 (10) | −0.0027 (12) |
| C2 | 0.0357 (13) | 0.0443 (15) | 0.0421 (14) | 0.0023 (11) | −0.0010 (10) | 0.0016 (12) |
| C3 | 0.0463 (15) | 0.0544 (17) | 0.0463 (15) | 0.0062 (13) | 0.0002 (11) | 0.0032 (13) |
| C4 | 0.0515 (17) | 0.0687 (19) | 0.0507 (15) | 0.0085 (14) | 0.0028 (12) | 0.0160 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0464 (16) | 0.0584 (19) | 0.0695 (19) | −0.0011 (13) | −0.0002 (13) | 0.0241 (15) |
| C6 | 0.0500 (15) | 0.0465 (16) | 0.0613 (17) | −0.0003 (12) | −0.0016 (13) | 0.0076 (13) |
| C7 | 0.0344 (14) | 0.0413 (15) | 0.0490 (14) | 0.0004 (11) | −0.0046 (11) | 0.0072 (12) |
| C8 | 0.0461 (14) | 0.0387 (15) | 0.0513 (15) | −0.0011 (11) | −0.0052 (12) | −0.0054 (12) |
| C9 | 0.0347 (14) | 0.0368 (15) | 0.0445 (13) | −0.0002 (10) | −0.0019 (11) | −0.0060 (11) |
| C10 | 0.0399 (14) | 0.0336 (13) | 0.0386 (13) | −0.0029 (11) | −0.0012 (10) | −0.0018 (11) |
| C11 | 0.0441 (14) | 0.0436 (15) | 0.0492 (15) | −0.0011 (12) | −0.0005 (11) | −0.0047 (12) |
| C12 | 0.0519 (16) | 0.0604 (18) | 0.0563 (17) | 0.0036 (13) | −0.0129 (13) | 0.0072 (15) |
| C13 | 0.075 (2) | 0.077 (2) | 0.0416 (15) | −0.0091 (16) | −0.0111 (14) | 0.0000 (15) |
| C14 | 0.0721 (18) | 0.0580 (18) | 0.0483 (16) | −0.0068 (15) | 0.0073 (14) | −0.0115 (14) |
| C15 | 0.0507 (15) | 0.0429 (15) | 0.0497 (15) | 0.0013 (12) | 0.0008 (12) | −0.0051 (13) |
| C16 | 0.0436 (14) | 0.0361 (14) | 0.0423 (13) | −0.0039 (11) | −0.0025 (11) | −0.0031 (12) |
| C17 | 0.0400 (13) | 0.0351 (14) | 0.0458 (14) | −0.0048 (11) | −0.0039 (11) | −0.0015 (11) |
| C18 | 0.0586 (15) | 0.0392 (15) | 0.0463 (15) | 0.0034 (13) | 0.0039 (12) | −0.0031 (12) |
| C19 | 0.0637 (17) | 0.0400 (15) | 0.0532 (16) | 0.0085 (12) | 0.0004 (13) | 0.0023 (13) |
| C20 | 0.0498 (15) | 0.0497 (16) | 0.0446 (14) | −0.0053 (13) | −0.0014 (12) | 0.0051 (13) |
| C21 | 0.0516 (16) | 0.0559 (17) | 0.0497 (16) | 0.0024 (14) | 0.0067 (12) | −0.0002 (13) |
| C22 | 0.0516 (16) | 0.0417 (15) | 0.0575 (16) | 0.0052 (12) | −0.0014 (13) | 0.0000 (13) |
| C23 | 0.0591 (18) | 0.075 (2) | 0.0546 (18) | 0.0052 (14) | 0.0030 (14) | 0.0043 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C16 | 1.380 (2) | C10—C11 | 1.387 (3) |
| N1—C1 | 1.385 (2) | C11—C12 | 1.382 (3) |
| N1—C9 | 1.416 (2) | C11—H11 | 0.9300 |
| N2—C16 | 1.314 (2) | C12—C13 | 1.371 (3) |
| N2—N3 | 1.379 (2) | C12—H12 | 0.9300 |
| N3—C1 | 1.318 (3) | C13—C14 | 1.362 (3) |
| N4—C23 | 1.133 (3) | C13—H13 | 0.9300 |
| C1—C2 | 1.426 (3) | C14—C15 | 1.377 (3) |
| C2—C3 | 1.398 (3) | C14—H14 | 0.9300 |
| C2—C7 | 1.404 (3) | C15—H15 | 0.9300 |
| C3—C4 | 1.372 (3) | C16—C17 | 1.467 (3) |
| C3—H3 | 0.9300 | C17—C22 | 1.387 (3) |
| C4—C5 | 1.386 (3) | C17—C18 | 1.389 (3) |
| C4—H4 | 0.9300 | C18—C19 | 1.379 (3) |
| C5—C6 | 1.374 (3) | C18—H18 | 0.9300 |
| C5—H5 | 0.9300 | C19—C20 | 1.384 (3) |
| C6—C7 | 1.398 (3) | C19—H19 | 0.9300 |
| C6—H6 | 0.9300 | C20—C21 | 1.381 (3) |
| C7—C8 | 1.437 (3) | C20—C23 | 1.445 (3) |
| C8—C9 | 1.342 (3) | C21—C22 | 1.382 (3) |
| C8—H8 | 0.9300 | C21—H21 | 0.9300 |
| C9—C10 | 1.481 (3) | C22—H22 | 0.9300 |
| C10—C15 | 1.384 (3) | | |
| | | | |
| C16—N1—C1 | 104.23 (17) | C12—C11—H11 | 120.1 |
| C16—N1—C9 | 133.97 (18) | C10—C11—H11 | 120.1 |

| | | | |
|---|---|---|---|
| C1—N1—C9 | 121.67 (19) | C13—C12—C11 | 120.5 (2) |
| C16—N2—N3 | 108.54 (17) | C13—C12—H12 | 119.7 |
| C1—N3—N2 | 107.01 (17) | C11—C12—H12 | 119.7 |
| N3—C1—N1 | 110.4 (2) | C14—C13—C12 | 120.1 (2) |
| N3—C1—C2 | 128.7 (2) | C14—C13—H13 | 119.9 |
| N1—C1—C2 | 120.8 (2) | C12—C13—H13 | 119.9 |
| C3—C2—C7 | 119.7 (2) | C13—C14—C15 | 120.1 (2) |
| C3—C2—C1 | 122.7 (2) | C13—C14—H14 | 120.0 |
| C7—C2—C1 | 117.6 (2) | C15—C14—H14 | 120.0 |
| C4—C3—C2 | 120.4 (2) | C14—C15—C10 | 120.7 (2) |
| C4—C3—H3 | 119.8 | C14—C15—H15 | 119.7 |
| C2—C3—H3 | 119.8 | C10—C15—H15 | 119.7 |
| C3—C4—C5 | 119.7 (2) | N2—C16—N1 | 109.78 (18) |
| C3—C4—H4 | 120.2 | N2—C16—C17 | 123.23 (19) |
| C5—C4—H4 | 120.2 | N1—C16—C17 | 126.94 (19) |
| C6—C5—C4 | 121.2 (2) | C22—C17—C18 | 118.8 (2) |
| C6—C5—H5 | 119.4 | C22—C17—C16 | 122.4 (2) |
| C4—C5—H5 | 119.4 | C18—C17—C16 | 118.8 (2) |
| C5—C6—C7 | 119.9 (2) | C19—C18—C17 | 120.6 (2) |
| C5—C6—H6 | 120.0 | C19—C18—H18 | 119.7 |
| C7—C6—H6 | 120.0 | C17—C18—H18 | 119.7 |
| C6—C7—C2 | 119.1 (2) | C18—C19—C20 | 119.9 (2) |
| C6—C7—C8 | 122.1 (2) | C18—C19—H19 | 120.1 |
| C2—C7—C8 | 118.6 (2) | C20—C19—H19 | 120.1 |
| C9—C8—C7 | 124.0 (2) | C21—C20—C19 | 120.2 (2) |
| C9—C8—H8 | 118.0 | C21—C20—C23 | 119.9 (2) |
| C7—C8—H8 | 118.0 | C19—C20—C23 | 119.9 (2) |
| C8—C9—N1 | 116.90 (19) | C20—C21—C22 | 119.7 (2) |
| C8—C9—C10 | 122.32 (19) | C20—C21—H21 | 120.2 |
| N1—C9—C10 | 120.61 (19) | C22—C21—H21 | 120.2 |
| C15—C10—C11 | 118.9 (2) | C21—C22—C17 | 120.8 (2) |
| C15—C10—C9 | 119.4 (2) | C21—C22—H22 | 119.6 |
| C11—C10—C9 | 121.49 (19) | C17—C22—H22 | 119.6 |
| C12—C11—C10 | 119.7 (2) | N4—C23—C20 | 179.2 (3) |

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| C16—N2—N3—C1 | 0.5 (2) | N1—C9—C10—C15 | −131.8 (2) |
| N2—N3—C1—N1 | 0.3 (2) | C8—C9—C10—C11 | −121.8 (2) |
| N2—N3—C1—C2 | −178.9 (2) | N1—C9—C10—C11 | 53.2 (3) |
| C16—N1—C1—N3 | −0.9 (2) | C15—C10—C11—C12 | 1.0 (3) |
| C9—N1—C1—N3 | 175.46 (16) | C9—C10—C11—C12 | 176.0 (2) |
| C16—N1—C1—C2 | 178.40 (18) | C10—C11—C12—C13 | −0.9 (3) |
| C9—N1—C1—C2 | −5.2 (3) | C11—C12—C13—C14 | −0.4 (4) |
| N3—C1—C2—C3 | −2.5 (3) | C12—C13—C14—C15 | 1.4 (4) |
| N1—C1—C2—C3 | 178.35 (17) | C13—C14—C15—C10 | −1.3 (4) |
| N3—C1—C2—C7 | 178.8 (2) | C11—C10—C15—C14 | 0.0 (3) |
| N1—C1—C2—C7 | −0.4 (3) | C9—C10—C15—C14 | −175.0 (2) |
| C7—C2—C3—C4 | 0.2 (3) | N3—N2—C16—N1 | −1.0 (2) |
| C1—C2—C3—C4 | −178.5 (2) | N3—N2—C16—C17 | 176.63 (18) |

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| C2—C3—C4—C5 | −0.8 (3) | C1—N1—C16—N2 | 1.2 (2) |
| C3—C4—C5—C6 | 0.4 (3) | C9—N1—C16—N2 | −174.51 (19) |
| C4—C5—C6—C7 | 0.7 (3) | C1—N1—C16—C17 | −176.38 (19) |
| C5—C6—C7—C2 | −1.2 (3) | C9—N1—C16—C17 | 7.9 (4) |
| C5—C6—C7—C8 | 174.57 (19) | N2—C16—C17—C22 | −120.5 (2) |
| C3—C2—C7—C6 | 0.8 (3) | N1—C16—C17—C22 | 56.7 (3) |
| C1—C2—C7—C6 | 179.55 (19) | N2—C16—C17—C18 | 57.8 (3) |
| C3—C2—C7—C8 | −175.16 (18) | N1—C16—C17—C18 | −125.0 (2) |
| C1—C2—C7—C8 | 3.6 (3) | C22—C17—C18—C19 | −3.0 (3) |
| C6—C7—C8—C9 | −177.2 (2) | C16—C17—C18—C19 | 178.6 (2) |
| C2—C7—C8—C9 | −1.5 (3) | C17—C18—C19—C20 | 1.4 (3) |
| C7—C8—C9—N1 | −3.9 (3) | C18—C19—C20—C21 | 0.7 (3) |
| C7—C8—C9—C10 | 171.32 (18) | C18—C19—C20—C23 | −178.3 (2) |
| C16—N1—C9—C8 | −177.6 (2) | C19—C20—C21—C22 | −1.2 (3) |
| C1—N1—C9—C8 | 7.3 (3) | C23—C20—C21—C22 | 177.8 (2) |
| C16—N1—C9—C10 | 7.0 (3) | C20—C21—C22—C17 | −0.4 (3) |
| C1—N1—C9—C10 | −168.06 (17) | C18—C17—C22—C21 | 2.5 (3) |
| C8—C9—C10—C15 | 53.1 (3) | C16—C17—C22—C21 | −179.2 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11···N3$^{i}$ | 0.93 | 2.50 | 3.418 (3) | 170 |

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