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# 1-(3,5-Dimethyl-1*H*-pyrazol-1-yl)-3-phenylisoquinoline

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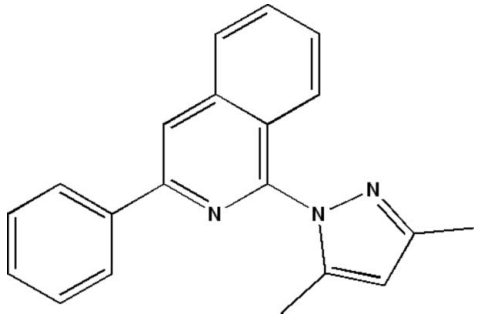
Key indicators: single-crystal X-ray study; $T$ = 290 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.052; $wR$ factor = 0.129; data-to-parameter ratio = 11.1.

The molecular conformation of the title compound, $C_{20}H_{17}N_3$, is stabilized by an intramolecular C—H···N interaction. The crystal structure shows intermolecular C—H···$\pi$ interactions. The dihedral angle between the isoquinoline unit and the phenyl ring is 11.42 (1)° whereas the isoquinoline unit and the pendent dimethyl pyrazole unit form a dihedral angle of 50.1 (4)°. Furthermore, the angle between the mean plane of the phenyl ring and the dimethyl pyrazole unit is 47.3 (6)°.

## Related literature

For general background to isoquinolines, see: Kametani *et al.* (1968); Broadhurst *et al.* (2001); Chao *et al.* (1999); Choudhury *et al.* (2002, 2006); Hathwar *et al.* (2008); Elguero *et al.* 2002).



## Experimental

### Crystal data

$C_{20}H_{17}N_3$
$M_r$ = 299.37
Orthorhombic, *Pbca*
$a$ = 18.3294 (14) Å
$b$ = 8.3139 (7) Å
$c$ = 21.6532 (17) Å
$V$ = 3299.7 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 290 K
0.18 × 0.11 × 0.07 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.949, $T_{max}$ = 0.995
22808 measured reflections
3065 independent reflections
2608 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.129
$S$ = 1.14
3065 reflections
276 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7···N3 | 0.94 (2) | 2.452 (17) | 3.001 (2) | 117.4 (13) |
| C4—H4···$Cg2^{i}$ | 0.91 (2) | 2.645 (17) | 3.325 (2) | 131.4 (13) |

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$. $Cg2$ is the centroid of the N1,C1–C3,C8,C9 ring.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2974).

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# supporting information

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## 1-(3,5-Dimethyl-1*H*-pyrazol-1-yl)-3-phenylisoquinoline

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### S1. Comment

Isoquinolines are an integral part of many naturally occurring fused heterocycles and find applications in synthetic and pharmaceutical chemistry (Kametani *et al.*, 1968). 3-substituted isoquinolines are of potent use in medicine, (Chao *et al.*, 1999) and in general, hydrazine derivatives can be used as medicaments (Broadhurst *et al.*, 2001). Choudhury *et al.* (2002, 2006) reported crystal structures of substituted isoquinolines while Hathwar *et al.* (2008) report the crystal structure of an isoquinolinyl diselenide. Similarly, compounds containing the pyrazole motif are being developed in a wide range of therapeutic areas including *CNS*, metabolic diseases and endocrine functions, and oncology (Elguero *et al.*, 2002). A number of pyrazole-containing compounds have been successfully commercialized, such as the blockbuster drugs Viagra, Celebrex, and Acomplia. In view of the diverse applications of this class of compounds, we report here the crystal structure of isoquinoline pyrazole, namely 1-(2,5-dimethyl-1*H*-pyrrol-1-yl)-3-phenylisoquinoline.

Although there are no intermolecular C—H···N hydrogen bonds, the molecules are linked by C—H···$\pi$ interactions.

In the absence of strong hydrogen-bond donors in (I), the crystal packing is controlled by the involvement of weak C—H..pi intermolecular interactions.

### S2. Experimental

The 3-phenylisoquinolinehydrazine, and the 1, 3-diketones namely acetylacetone, were taken in ethanol (1:1 ratio) and refluxed under nitrogen overnight. Then the reaction mass was quenched with water, extracted with ethylacetate, washed, dried, concentrated and purified by column chromatography to get titlted compound, (I). Single crystals of the title compound were obtained *via* recrystalization from a dichloromethane solution

### S3. Refinement

All the H atoms in (I) were positioned geometrically and refined using a riding model with C—H bond lenghts of 0.93 Å and 0.97 Å for aromatic and for methylene H atoms respectively and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all carbon bound H atoms.

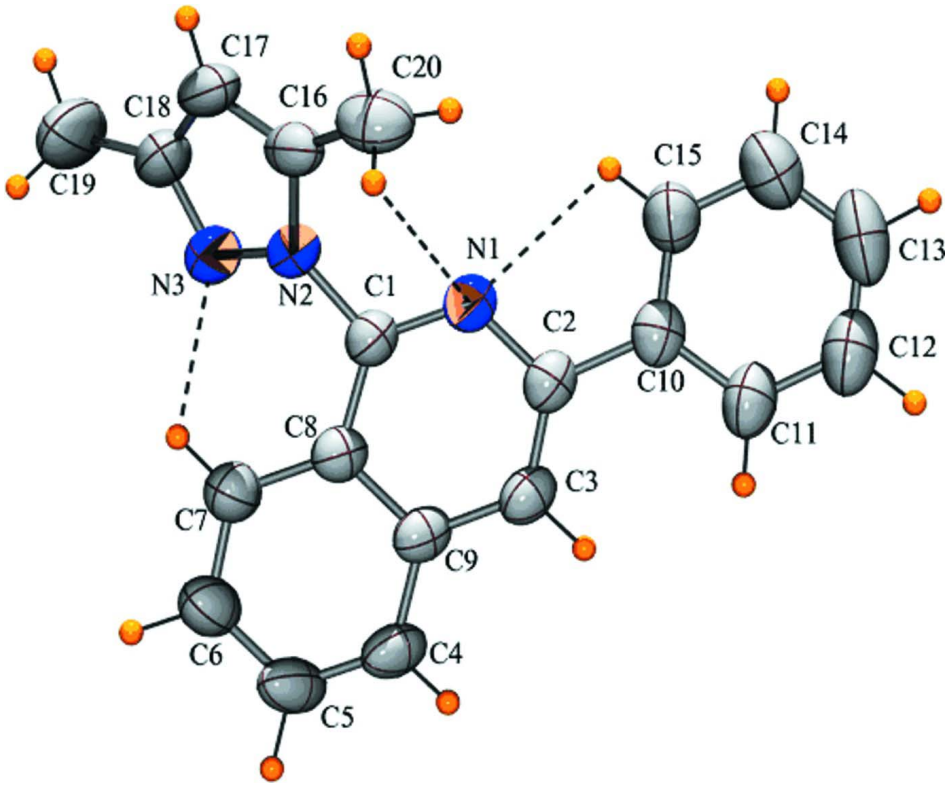


**Figure 1**

*ORTEP* diagram of the asymmetric unit of (I) with 50% probability displacement ellipsoids.

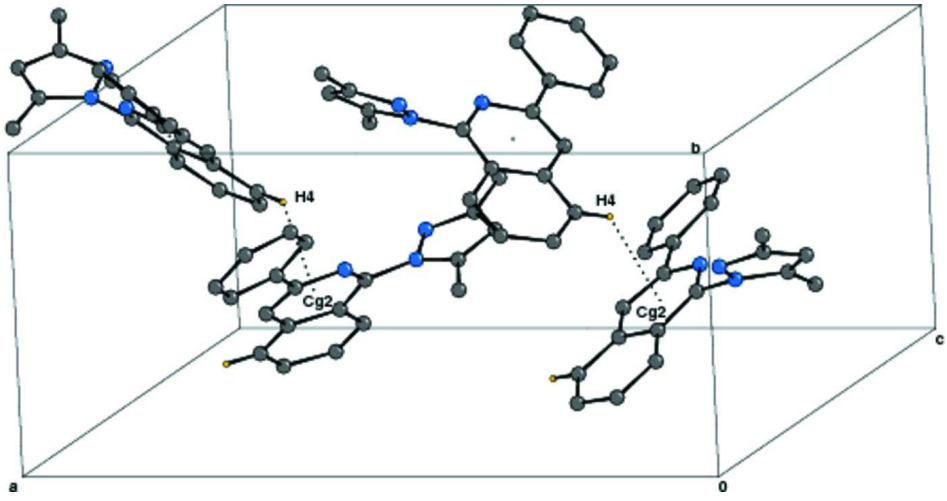


**Figure 2**

A packing excerpt from the crystal with dotted lines indicating intermolecular C—H···$\pi$ hydrogen bonds. H atoms not involved in the interactions are omitted for clarity.

**1-(3,5-Dimethyl-1H</>-pyrazol-1-yl)-3-phenylisoquinoline**

*Crystal data*

$C_{20}H_{17}N_3$
$M_r = 299.37$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 18.3294\ (14)$ Å
$b = 8.3139\ (7)$ Å
$c = 21.6532\ (17)$ Å
$V = 3299.7\ (5)$ Å$^3$
$Z = 8$
$F(000) = 1264$
$D_x = 1.205$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1248 reflections
$\theta = 2.2–27.2°$
$\mu = 0.07$ mm$^{-1}$
$T = 290$ K
Block, colorless
0.18 × 0.11 × 0.07 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.949$, $T_{max} = 0.995$
22808 measured reflections
3065 independent reflections
2608 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.9°$
$h = -22\rightarrow20$
$k = -10\rightarrow10$
$l = -26\rightarrow24$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.129$
$S = 1.14$
3065 reflections
276 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.6765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ 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.

**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 | 0.09848 (7) | 0.53396 (16) | 0.26708 (6) | 0.0490 (4) |
| N2 | 0.02198 (7) | 0.52682 (18) | 0.18301 (6) | 0.0538 (4) |
| C1 | 0.08768 (9) | 0.47659 (19) | 0.21175 (7) | 0.0470 (4) |
| C8 | 0.13594 (9) | 0.37101 (19) | 0.18015 (7) | 0.0477 (4) |
| C3 | 0.21303 (10) | 0.3989 (2) | 0.27066 (8) | 0.0525 (4) |

| | | | | |
|---|---|---|---|---|
| C9 | 0.20196 (9) | 0.3351 (2) | 0.21115 (8) | 0.0491 (4) |
| C2 | 0.16088 (9) | 0.4924 (2) | 0.29813 (8) | 0.0485 (4) |
| C10 | 0.16626 (9) | 0.5586 (2) | 0.36145 (8) | 0.0533 (4) |
| C4 | 0.25285 (11) | 0.2347 (2) | 0.18064 (9) | 0.0611 (5) |
| C16 | −0.04605 (9) | 0.5383 (2) | 0.20820 (9) | 0.0555 (5) |
| C7 | 0.12169 (11) | 0.3011 (2) | 0.12208 (8) | 0.0597 (5) |
| N3 | 0.02521 (8) | 0.5925 (2) | 0.12480 (7) | 0.0677 (5) |
| C20 | −0.06494 (13) | 0.4719 (3) | 0.26970 (12) | 0.0742 (6) |
| C5 | 0.23812 (12) | 0.1701 (3) | 0.12503 (9) | 0.0705 (6) |
| C11 | 0.22045 (12) | 0.5099 (3) | 0.40250 (9) | 0.0673 (6) |
| C15 | 0.11577 (12) | 0.6709 (3) | 0.38203 (9) | 0.0698 (6) |
| C6 | 0.17167 (12) | 0.2015 (3) | 0.09549 (10) | 0.0699 (6) |
| C12 | 0.22252 (14) | 0.5691 (3) | 0.46184 (10) | 0.0819 (7) |
| C18 | −0.04247 (12) | 0.6423 (3) | 0.11454 (9) | 0.0723 (6) |
| C13 | 0.17137 (16) | 0.6770 (3) | 0.48194 (11) | 0.0876 (8) |
| C17 | −0.08729 (12) | 0.6106 (3) | 0.16449 (10) | 0.0700 (6) |
| C14 | 0.11810 (15) | 0.7294 (3) | 0.44162 (11) | 0.0855 (7) |
| C19 | −0.06113 (15) | 0.7207 (4) | 0.05432 (11) | 0.1147 (10) |
| H19A | −0.0312 | 0.8144 | 0.0487 | 0.172* |
| H19B | −0.1116 | 0.7517 | 0.0545 | 0.172* |
| H19C | −0.0526 | 0.6464 | 0.0212 | 0.172* |
| H3 | 0.2583 (10) | 0.378 (2) | 0.2919 (8) | 0.064 (5)* |
| H7 | 0.0783 (10) | 0.330 (2) | 0.1015 (8) | 0.070 (6)* |
| H4 | 0.2958 (10) | 0.212 (2) | 0.2010 (9) | 0.065 (5)* |
| H11 | 0.2580 (13) | 0.431 (3) | 0.3893 (10) | 0.090 (7)* |
| H5 | 0.2750 (11) | 0.100 (3) | 0.1032 (9) | 0.080 (6)* |
| H15 | 0.0784 (11) | 0.712 (3) | 0.3537 (9) | 0.079 (6)* |
| H20C | −0.1161 (15) | 0.482 (3) | 0.2777 (10) | 0.106 (8)* |
| H17 | −0.1358 (12) | 0.633 (2) | 0.1678 (9) | 0.073 (6)* |
| H20B | −0.0531 (14) | 0.356 (4) | 0.2713 (12) | 0.128 (10)* |
| H14 | 0.0827 (11) | 0.809 (3) | 0.4543 (10) | 0.083 (7)* |
| H12 | 0.2612 (13) | 0.529 (3) | 0.4907 (11) | 0.104 (8)* |
| H20A | −0.0422 (13) | 0.531 (3) | 0.3038 (11) | 0.098 (8)* |
| H6 | 0.1605 (11) | 0.153 (3) | 0.0533 (11) | 0.090 (7)* |
| H13 | 0.1701 (12) | 0.718 (3) | 0.5233 (12) | 0.099 (8)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0454 (8) | 0.0533 (8) | 0.0483 (8) | −0.0005 (6) | −0.0008 (6) | 0.0040 (6) |
| N2 | 0.0449 (8) | 0.0652 (9) | 0.0513 (8) | 0.0098 (7) | −0.0043 (6) | −0.0032 (7) |
| C1 | 0.0424 (9) | 0.0510 (9) | 0.0474 (9) | 0.0001 (7) | −0.0008 (7) | 0.0054 (7) |
| C8 | 0.0459 (9) | 0.0484 (9) | 0.0489 (9) | 0.0017 (7) | 0.0051 (7) | 0.0088 (7) |
| C3 | 0.0449 (9) | 0.0588 (10) | 0.0540 (10) | 0.0024 (8) | −0.0011 (8) | 0.0162 (8) |
| C9 | 0.0457 (9) | 0.0503 (9) | 0.0512 (10) | 0.0033 (7) | 0.0052 (7) | 0.0168 (7) |
| C2 | 0.0468 (9) | 0.0506 (9) | 0.0480 (9) | −0.0056 (7) | −0.0009 (7) | 0.0118 (7) |
| C10 | 0.0545 (10) | 0.0578 (10) | 0.0478 (10) | −0.0113 (8) | −0.0001 (8) | 0.0106 (8) |
| C4 | 0.0567 (11) | 0.0659 (11) | 0.0607 (12) | 0.0191 (9) | 0.0073 (9) | 0.0213 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0437 (9) | 0.0549 (10) | 0.0679 (12) | 0.0022 (8) | −0.0008 (8) | −0.0161 (9) |
| C7 | 0.0632 (12) | 0.0634 (11) | 0.0524 (11) | 0.0101 (9) | −0.0005 (9) | 0.0026 (9) |
| N3 | 0.0647 (10) | 0.0857 (12) | 0.0528 (9) | 0.0237 (9) | −0.0041 (7) | 0.0024 (8) |
| C20 | 0.0531 (13) | 0.0783 (16) | 0.0912 (17) | −0.0012 (11) | 0.0162 (12) | −0.0037 (13) |
| C5 | 0.0844 (15) | 0.0722 (13) | 0.0550 (12) | 0.0320 (11) | 0.0164 (11) | 0.0138 (10) |
| C11 | 0.0665 (13) | 0.0829 (14) | 0.0526 (12) | −0.0092 (11) | −0.0073 (9) | 0.0133 (10) |
| C15 | 0.0766 (14) | 0.0766 (13) | 0.0563 (12) | −0.0002 (11) | −0.0052 (10) | −0.0015 (10) |
| C6 | 0.0863 (15) | 0.0710 (13) | 0.0524 (11) | 0.0241 (11) | 0.0046 (10) | 0.0018 (10) |
| C12 | 0.0833 (16) | 0.1038 (18) | 0.0586 (13) | −0.0167 (14) | −0.0144 (12) | 0.0141 (13) |
| C18 | 0.0707 (13) | 0.0816 (14) | 0.0647 (12) | 0.0302 (11) | −0.0169 (10) | −0.0101 (10) |
| C13 | 0.114 (2) | 0.0989 (18) | 0.0499 (13) | −0.0335 (16) | −0.0056 (13) | −0.0015 (12) |
| C17 | 0.0485 (11) | 0.0761 (13) | 0.0853 (15) | 0.0197 (10) | −0.0127 (10) | −0.0192 (11) |
| C14 | 0.1017 (18) | 0.0896 (16) | 0.0651 (14) | −0.0013 (15) | 0.0035 (13) | −0.0127 (12) |
| C19 | 0.117 (2) | 0.149 (3) | 0.0785 (16) | 0.065 (2) | −0.0211 (15) | 0.0087 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.305 (2) | C20—H20C | 0.96 (3) |
| N1—C2 | 1.371 (2) | C20—H20B | 0.99 (3) |
| N2—C16 | 1.364 (2) | C20—H20A | 0.98 (3) |
| N2—N3 | 1.375 (2) | C5—C6 | 1.400 (3) |
| N2—C1 | 1.418 (2) | C5—H5 | 1.01 (2) |
| C1—C8 | 1.422 (2) | C11—C12 | 1.376 (3) |
| C8—C7 | 1.410 (2) | C11—H11 | 1.00 (2) |
| C8—C9 | 1.416 (2) | C15—C14 | 1.380 (3) |
| C3—C2 | 1.368 (2) | C15—H15 | 0.98 (2) |
| C3—C9 | 1.408 (2) | C6—H6 | 1.02 (2) |
| C3—H3 | 0.966 (18) | C12—C13 | 1.369 (4) |
| C9—C4 | 1.416 (2) | C12—H12 | 1.00 (3) |
| C2—C10 | 1.481 (2) | C18—C17 | 1.383 (3) |
| C10—C15 | 1.388 (3) | C18—C19 | 1.498 (3) |
| C10—C11 | 1.393 (3) | C13—C14 | 1.380 (3) |
| C4—C5 | 1.346 (3) | C13—H13 | 0.96 (2) |
| C4—H4 | 0.922 (18) | C17—H17 | 0.91 (2) |
| C16—C17 | 1.353 (3) | C14—H14 | 0.97 (2) |
| C16—C20 | 1.482 (3) | C19—H19A | 0.9600 |
| C7—C6 | 1.362 (3) | C19—H19B | 0.9600 |
| C7—H7 | 0.943 (19) | C19—H19C | 0.9600 |
| N3—C18 | 1.326 (2) | | |
| | | | |
| C1—N1—C2 | 119.00 (14) | H20C—C20—H20A | 103.7 (19) |
| C16—N2—N3 | 112.22 (14) | H20B—C20—H20A | 112 (2) |
| C16—N2—C1 | 128.39 (15) | C4—C5—C6 | 120.56 (19) |
| N3—N2—C1 | 118.85 (13) | C4—C5—H5 | 121.0 (11) |
| N1—C1—N2 | 115.09 (14) | C6—C5—H5 | 118.4 (11) |
| N1—C1—C8 | 124.98 (15) | C12—C11—C10 | 120.7 (2) |
| N2—C1—C8 | 119.92 (15) | C12—C11—H11 | 119.0 (13) |
| C7—C8—C9 | 119.62 (16) | C10—C11—H11 | 120.2 (13) |

| | | | |
|---|---|---|---|
| C7—C8—C1 | 124.66 (16) | C14—C15—C10 | 121.1 (2) |
| C9—C8—C1 | 115.72 (15) | C14—C15—H15 | 119.0 (12) |
| C2—C3—C9 | 120.75 (16) | C10—C15—H15 | 119.9 (12) |
| C2—C3—H3 | 119.8 (11) | C7—C6—C5 | 120.4 (2) |
| C9—C3—H3 | 119.4 (11) | C7—C6—H6 | 119.0 (12) |
| C3—C9—C4 | 123.67 (16) | C5—C6—H6 | 120.6 (12) |
| C3—C9—C8 | 118.52 (15) | C13—C12—C11 | 120.8 (2) |
| C4—C9—C8 | 117.80 (17) | C13—C12—H12 | 120.2 (14) |
| C3—C2—N1 | 120.85 (16) | C11—C12—H12 | 118.9 (15) |
| C3—C2—C10 | 124.57 (15) | N3—C18—C17 | 111.41 (18) |
| N1—C2—C10 | 114.57 (15) | N3—C18—C19 | 119.7 (2) |
| C15—C10—C11 | 117.79 (19) | C17—C18—C19 | 128.89 (19) |
| C15—C10—C2 | 120.19 (16) | C12—C13—C14 | 119.4 (2) |
| C11—C10—C2 | 122.00 (18) | C12—C13—H13 | 123.1 (14) |
| C5—C4—C9 | 121.39 (19) | C14—C13—H13 | 117.5 (14) |
| C5—C4—H4 | 121.1 (12) | C16—C17—C18 | 107.44 (18) |
| C9—C4—H4 | 117.5 (12) | C16—C17—H17 | 125.4 (13) |
| C17—C16—N2 | 105.19 (18) | C18—C17—H17 | 127.1 (13) |
| C17—C16—C20 | 131.6 (2) | C15—C14—C13 | 120.1 (3) |
| N2—C16—C20 | 123.14 (17) | C15—C14—H14 | 119.1 (13) |
| C6—C7—C8 | 120.20 (19) | C13—C14—H14 | 120.8 (13) |
| C6—C7—H7 | 121.4 (12) | C18—C19—H19A | 109.5 |
| C8—C7—H7 | 118.3 (12) | C18—C19—H19B | 109.5 |
| C18—N3—N2 | 103.72 (16) | H19A—C19—H19B | 109.5 |
| C16—C20—H20C | 111.2 (14) | C18—C19—H19C | 109.5 |
| C16—C20—H20B | 110.1 (16) | H19A—C19—H19C | 109.5 |
| H20C—C20—H20B | 107 (2) | H19B—C19—H19C | 109.5 |
| C16—C20—H20A | 112.9 (14) | | |

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| C2—N1—C1—N2 | −179.60 (14) | N3—N2—C16—C17 | 1.0 (2) |
| C2—N1—C1—C8 | 0.5 (2) | C1—N2—C16—C17 | 172.43 (17) |
| C16—N2—C1—N1 | −43.2 (2) | N3—N2—C16—C20 | 177.88 (18) |
| N3—N2—C1—N1 | 127.74 (16) | C1—N2—C16—C20 | −10.7 (3) |
| C16—N2—C1—C8 | 136.70 (18) | C9—C8—C7—C6 | −1.0 (3) |
| N3—N2—C1—C8 | −52.4 (2) | C1—C8—C7—C6 | 179.82 (18) |
| N1—C1—C8—C7 | 175.60 (16) | C16—N2—N3—C18 | −0.9 (2) |
| N2—C1—C8—C7 | −4.3 (2) | C1—N2—N3—C18 | −173.20 (16) |
| N1—C1—C8—C9 | −3.6 (2) | C9—C4—C5—C6 | 0.4 (3) |
| N2—C1—C8—C9 | 176.55 (14) | C15—C10—C11—C12 | 1.4 (3) |
| C2—C3—C9—C4 | −178.55 (16) | C2—C10—C11—C12 | −177.56 (18) |
| C2—C3—C9—C8 | 0.6 (2) | C11—C10—C15—C14 | −1.5 (3) |
| C7—C8—C9—C3 | −176.34 (15) | C2—C10—C15—C14 | 177.43 (19) |
| C1—C8—C9—C3 | 2.9 (2) | C8—C7—C6—C5 | −1.2 (3) |
| C7—C8—C9—C4 | 2.8 (2) | C4—C5—C6—C7 | 1.5 (3) |
| C1—C8—C9—C4 | −177.96 (15) | C10—C11—C12—C13 | 0.1 (3) |
| C9—C3—C2—N1 | −3.8 (2) | N2—N3—C18—C17 | 0.4 (2) |
| C9—C3—C2—C10 | 177.19 (15) | N2—N3—C18—C19 | −179.4 (2) |
| C1—N1—C2—C3 | 3.3 (2) | C11—C12—C13—C14 | −1.4 (4) |

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| C1—N1—C2—C10 | −177.61 (14) | N2—C16—C17—C18 | −0.7 (2) |
| C3—C2—C10—C15 | 170.61 (17) | C20—C16—C17—C18 | −177.2 (2) |
| N1—C2—C10—C15 | −8.4 (2) | N3—C18—C17—C16 | 0.2 (3) |
| C3—C2—C10—C11 | −10.5 (3) | C19—C18—C17—C16 | 180.0 (2) |
| N1—C2—C10—C11 | 170.48 (16) | C10—C15—C14—C13 | 0.2 (4) |
| C3—C9—C4—C5 | 176.59 (18) | C12—C13—C14—C15 | 1.3 (4) |
| C8—C9—C4—C5 | −2.5 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···N3 | 0.94 (2) | 2.452 (17) | 3.001 (2) | 117.4 (13) |
| C4—H4···*Cg*2$^{i}$ | 0.91 (2) | 2.645 (17) | 3.325 (2) | 131.4 (13) |

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