Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

P. Manivel,[a] Venkatesha R. Hathwar,[b] T. Maiyalagan,[a] V. Krishnakumar[a] and F. Nawaz Khan[a]*

[a]Chemistry Division, School of Science and Humanities, VIT University, Vellore 632 014, Tamil Nadu, India, and [b]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India
Correspondence e-mail: nawaz_f@yahoo.co.in

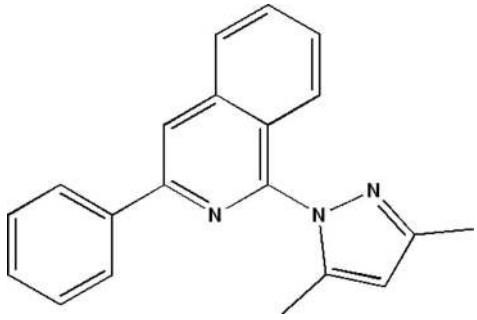
Received 17 June 2009; accepted 27 June 2009

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(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···π 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
μ = 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).

We thank the Department of Science and Technology, India, for use of the CCD facility set up under the IRHPA–DST program at IISc. We thank Professor T. N. Guru Row, IISc, Bangalore, for useful crystallographic discussions. FNK thanks the DST for Fast Track Proposal funding.

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

References

Broadhurst, M. D., Michael, J. J., William, H. W. & Daryl, S. (2001). US Patent No. 6 235 787.
Bruker (2004). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chao, Q., Deng, L., Shih, H., Leoni, L. M., Genini, D., Carson, D. A. & Cottam, H. B. (1999). *J. Med. Chem.* **2**, 3860–3873.
Choudhury, A. R. & Guru Row, T. N. (2006). *CrystEngComm*, **8**, 265–274.
Choudhury, A. R., Urs, U. K., Guru Row, T. N. & Nagarajan, K. (2002). *J. Mol. Struct.* **605**, 71–77.
Elguero, J., Goya, P., Jagerovic, N. & Silva, A. M. S. (2002). *Targets in Heterocyclic Systems*, Vol. 6, pp. 52–98. Rome: Italian Society of Chemistry.
Hathwar, V. R., Prabakaran, K., Subashini, R., Manivel, P. & Khan, F. N. (2008). *Acta Cryst.* E**64**, o2295.
Kametani, T. (1968). *The Chemistry of the Isoquinoline Alkaloids*. Tokyo: Hirokawa; Amsterdam: Elsevier.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Watkin, D. J., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

supporting information

Acta Cryst. (2009). E**65**, o1798 [doi:10.1107/S1600536809024842]

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

P. Manivel, Venkatesha R. Hathwar, T. Maiyalagan, V. Krishnakumar and F. Nawaz Khan

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···π 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) = 1.2U_{eq}(C) for all carbon bound H atoms.

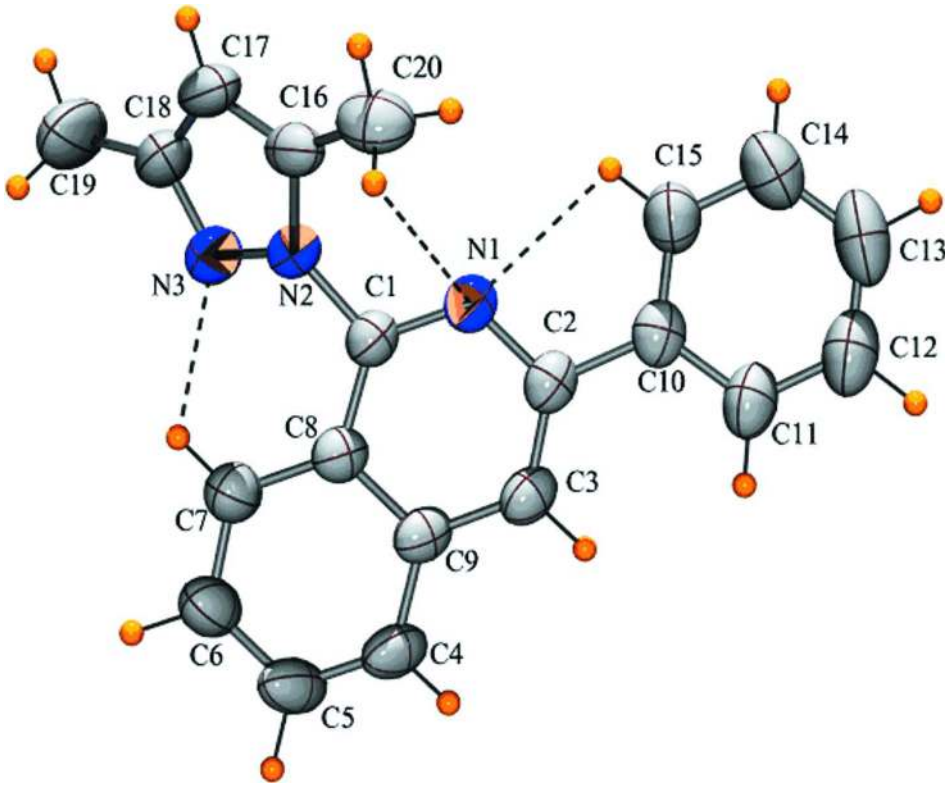


Figure 1

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

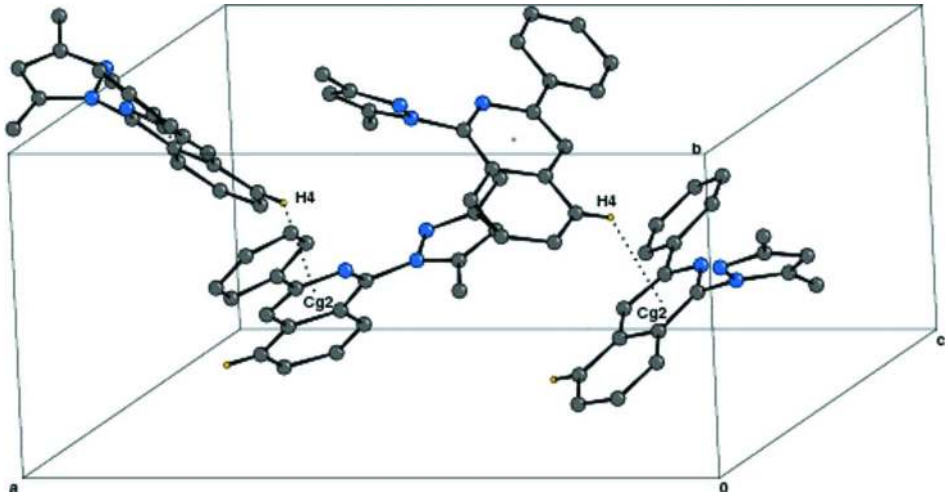


Figure 2

A packing excerpt from the crystal with dotted lines indicating intermolecular C—H···π 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
φ and ω 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)		

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)

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*.