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5-Methyl-4-(3-methyl-1-phenyl-1*H*-pyrazol-4-yl)-2-phenyl-2,3-dihydro-1*H*-pyrazol-3-one

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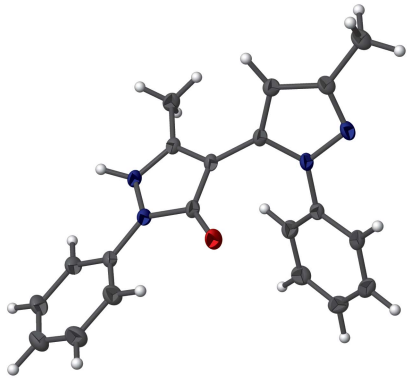
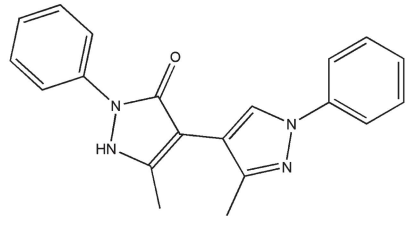
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{18}N_4O$, the dihedral angle between the pyrazole and pyrazolone rings is 69.35 (3)° and an intramolecular C—H···O hydrogen bond encloses an $R_2^2(6)$ ring. In the crystal, the packing features N—H···O and C—H···O hydrogen bonds and C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Materials containing pyrazolone ring systems represent an important class of compounds, not only for their theoretical interest, but also because of their pharmaceutical applications. These include use as anti-inflammatory, analgesic, antipyretic (El-Sayed & El-Ashmawey, 1998) and hypoglycemic agents (Das *et al.*, 2008). They also have fungicidal (Singh & Singh, 1991) and antimicrobial properties (Sahu *et al.*, 2007) and some have been tested as potential cardiovascular drugs (Higashi *et al.*, 2006). In the past year, research has focused on existing molecules and their modifications in order to reduce side effects and to explore other pharmacological and biological effects. As part of our work in this area, the synthesis and structure of the title compound, Fig. 1, are described here.

An intramolecular C6—H6···O1 hydrogen bond encloses an $R_2^2(6)$ ring and affects the conformation of the phenylpyrazalone segment of the molecule. The dihedral angle between the C1–C6 phenyl ring and the N1/N2/C7–C9 pyrazolone ring is 16.56 (6)° while that between the pyrazolone and pyrazole rings is 69.35 (3)°. The corresponding dihedral angle between the C15–C20 phenyl ring and the N3/N4/C11–C13 pyrazole ring is 39.72 (5)°.

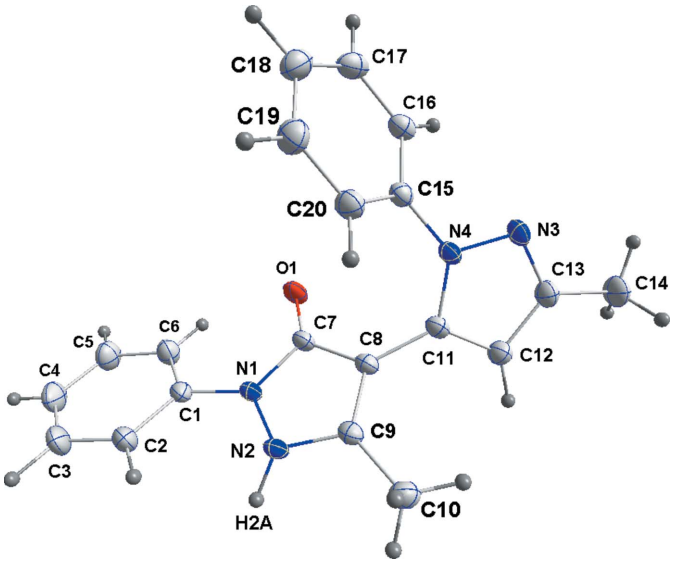


Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids.

In the crystal the strongest intermolecular interaction is the N2—H2*A*···O1^{i} hydrogen bond (Table 1, Figs. 2 and 3. This is supported by a C2—H2···O1^{i} hydrogen bond and together they link molecules into chains along the *c*-axis direction. The packing is further facilitated by four C—H···π(ring) interactions, as illustrated in Fig. 3.

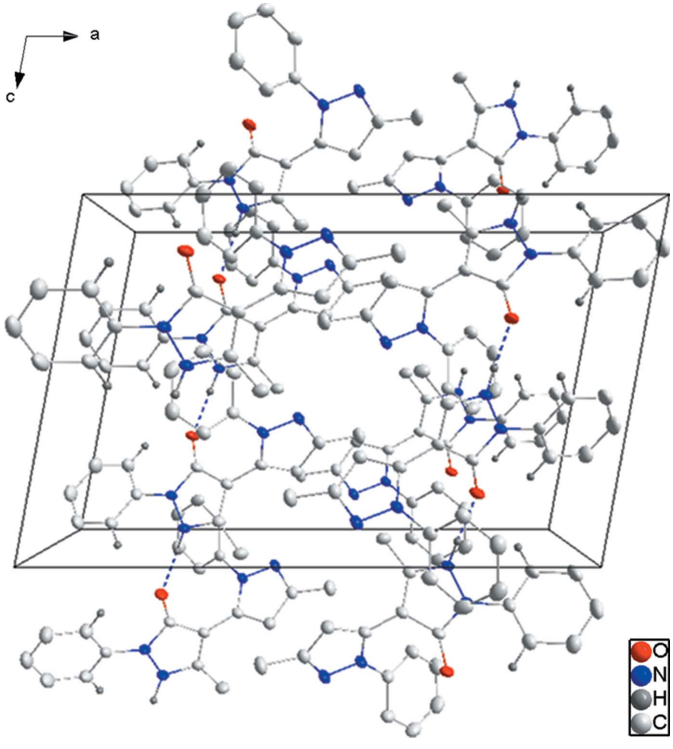


Figure 2
Packing viewed along the *b* axis with intermolecular N—H···O hydrogen bonds shown as dotted lines.

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

*Cg*2, *Cg*3 and *Cg*4 are the centroids of the N3/N4/C11–C13, C1–C6 and C15–C20 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.948 (17)	1.788 (17)	2.7326 (12)	173.8 (15)
C2—H2···O1^{i}	0.991 (16)	2.490 (16)	3.2058 (15)	128.8 (12)
C6—H6···O1	0.976 (16)	2.282 (16)	2.9210 (15)	122.2 (12)
C5—H5···*Cg*3^{ii}	0.997 (17)	2.706 (16)	3.6201 (15)	153.0 (12)
C10—H10*A*···*Cg*2^{iii}	0.94 (2)	2.79 (2)	3.5373 (13)	136.5 (18)
C10—H10*B*···*Cg*4^{iv}	0.98 (2)	2.83 (2)	3.7117 (14)	150.3 (17)
C14—H14*B*···*Cg*2^{v}	0.99 (2)	2.77 (2)	3.6861 (16)	154.9 (16)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{18}N_4O$
M_r	330.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	18.2838 (13), 7.7956 (6), 11.8081 (8)
β (°)	100.393 (3)
V (Å^3)	1655.4 (2)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.68
Crystal size (mm)	0.22 × 0.18 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.94
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12696, 3308, 3049
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.093, 1.05
No. of reflections	3308
No. of parameters	299
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.18

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

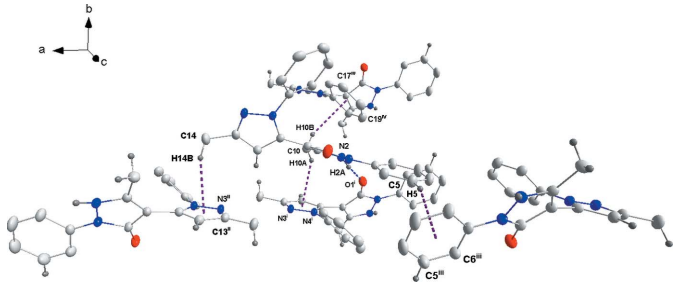


Figure 3
Details of the C—H···π(ring) interactions (purple dotted lines) and the N—H···O hydrogen bond (blue dotted line) [symmetry codes: (i) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (iii) $-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (iv) $x, \frac{3}{2}-y, \frac{1}{2}+z$].

Synthesis and crystallization

To a solution of dehydroacetic acid (0.168 g, 1 mmol), copper(II) sulfate pentahydrate (0.249 g, 1 mmol) was added as a catalyst together with a solution of phenylhydrazine (0.099 ml, 1 mmol) in absolute ethanol (30 ml). The reaction mixture was stirred for 3 h at 351 K. Colorless block-like crystals were obtained after cooling the reaction to 298 K (yield = 67%; m.p. = 523 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170853 [https://doi.org/10.1107/S2414314617008537]

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Crystal data

$C_{20}H_{18}N_4O$
M_r = 330.38
Monoclinic, $P2_1/c$
a = 18.2838 (13) Å
b = 7.7956 (6) Å
c = 11.8081 (8) Å
β = 100.393 (3)°
V = 1655.4 (2) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.326 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9980 reflections
θ = 2.5–74.7°
μ = 0.68 mm^{-1}
T = 150 K
Block, colourless
0.22 × 0.18 × 0.10 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.86, T_{max} = 0.94
12696 measured reflections
3308 independent reflections
3049 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 74.7°, θ_{min} = 4.9°
h = −22→21
k = −9→8
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.093
S = 1.05
3308 reflections
299 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.5397P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0106 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.21528 (5)	0.21776 (12)	0.67688 (6)	0.0285 (2)
N1	0.19857 (5)	0.27643 (12)	0.86378 (7)	0.0197 (2)
N2	0.24072 (5)	0.35100 (12)	0.96039 (7)	0.0201 (2)
H2A	0.2330 (9)	0.319 (2)	1.0348 (14)	0.038 (4)*
N3	0.43012 (5)	0.45260 (12)	0.61521 (8)	0.0230 (2)
N4	0.36552 (5)	0.46088 (12)	0.65819 (8)	0.0200 (2)
C1	0.12381 (6)	0.22855 (14)	0.86357 (9)	0.0205 (2)
C2	0.08809 (7)	0.28638 (17)	0.95115 (10)	0.0284 (3)
H2	0.1155 (9)	0.361 (2)	1.0123 (14)	0.037 (4)*
C3	0.01570 (7)	0.2340 (2)	0.95303 (12)	0.0366 (3)
H3	−0.0102 (10)	0.275 (2)	1.0193 (16)	0.053 (5)*
C4	−0.02153 (7)	0.12675 (19)	0.86882 (12)	0.0368 (3)
H4	−0.0718 (10)	0.086 (2)	0.8707 (15)	0.046 (4)*
C5	0.01404 (7)	0.07181 (18)	0.78120 (12)	0.0339 (3)
H5	−0.0117 (9)	−0.007 (2)	0.7206 (14)	0.045 (4)*
C6	0.08652 (7)	0.12168 (16)	0.77770 (10)	0.0279 (3)
H6	0.1116 (9)	0.084 (2)	0.7157 (13)	0.034 (4)*
C7	0.23913 (6)	0.27631 (14)	0.77497 (9)	0.0203 (2)
C8	0.30915 (6)	0.35407 (13)	0.82245 (9)	0.0193 (2)
C9	0.30790 (6)	0.39215 (13)	0.93601 (9)	0.0194 (2)
C10	0.36562 (7)	0.46954 (16)	1.02632 (10)	0.0260 (3)
H10A	0.3676 (12)	0.418 (3)	1.099 (2)	0.080 (7)*
H10B	0.3533 (12)	0.589 (3)	1.0386 (18)	0.072 (6)*
H10C	0.4149 (13)	0.468 (3)	1.0048 (19)	0.073 (6)*
C11	0.37120 (6)	0.37597 (14)	0.76121 (9)	0.0196 (2)
C12	0.44289 (6)	0.31276 (15)	0.78571 (10)	0.0229 (2)
H12	0.4657 (9)	0.2424 (19)	0.8532 (13)	0.033 (4)*
C13	0.47676 (6)	0.36365 (15)	0.69282 (10)	0.0234 (2)
C14	0.55367 (7)	0.32664 (19)	0.67266 (12)	0.0324 (3)
H14A	0.5929 (12)	0.389 (3)	0.7326 (19)	0.071 (6)*
H14B	0.5649 (12)	0.203 (3)	0.6810 (18)	0.072 (6)*
H14C	0.5598 (10)	0.364 (2)	0.5934 (15)	0.046 (5)*
C15	0.30487 (6)	0.55447 (13)	0.59520 (9)	0.0202 (2)
C16	0.29122 (7)	0.54406 (14)	0.47580 (9)	0.0237 (2)
H16	0.3224 (8)	0.4722 (18)	0.4379 (12)	0.028 (4)*

C17	0.23177 (7)	0.63393 (16)	0.41357 (10)	0.0291 (3)
H17	0.2205 (8)	0.622 (2)	0.3278 (14)	0.035 (4)*
C18	0.18726 (7)	0.73638 (16)	0.46884 (12)	0.0322 (3)
H18	0.1438 (10)	0.800 (2)	0.4241 (15)	0.045 (4)*
C19	0.20264 (7)	0.74963 (17)	0.58769 (12)	0.0316 (3)
H19	0.1711 (9)	0.821 (2)	0.6277 (14)	0.045 (4)*
C20	0.26126 (7)	0.65856 (15)	0.65170 (10)	0.0253 (3)
H20	0.2732 (8)	0.6686 (19)	0.7353 (13)	0.031 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0274 (4)	0.0447 (5)	0.0145 (4)	−0.0073 (4)	0.0070 (3)	−0.0068 (3)
N1	0.0204 (5)	0.0261 (5)	0.0134 (4)	−0.0009 (3)	0.0052 (3)	−0.0016 (3)
N2	0.0233 (5)	0.0250 (5)	0.0127 (4)	−0.0012 (4)	0.0050 (4)	−0.0012 (3)
N3	0.0205 (5)	0.0274 (5)	0.0239 (5)	−0.0001 (4)	0.0111 (4)	0.0004 (4)
N4	0.0203 (5)	0.0234 (5)	0.0184 (4)	0.0008 (3)	0.0087 (4)	0.0019 (3)
C1	0.0193 (5)	0.0243 (5)	0.0189 (5)	0.0019 (4)	0.0058 (4)	0.0043 (4)
C2	0.0238 (6)	0.0416 (7)	0.0211 (5)	0.0027 (5)	0.0078 (5)	0.0000 (5)
C3	0.0257 (6)	0.0572 (9)	0.0302 (6)	0.0025 (6)	0.0136 (5)	0.0023 (6)
C4	0.0228 (6)	0.0478 (8)	0.0416 (7)	−0.0027 (5)	0.0109 (5)	0.0065 (6)
C5	0.0261 (6)	0.0376 (7)	0.0380 (7)	−0.0055 (5)	0.0058 (5)	−0.0031 (6)
C6	0.0252 (6)	0.0320 (6)	0.0277 (6)	−0.0014 (5)	0.0080 (5)	−0.0036 (5)
C7	0.0226 (5)	0.0247 (5)	0.0150 (5)	0.0010 (4)	0.0069 (4)	0.0009 (4)
C8	0.0218 (5)	0.0214 (5)	0.0158 (5)	−0.0001 (4)	0.0063 (4)	0.0015 (4)
C9	0.0225 (5)	0.0192 (5)	0.0171 (5)	0.0008 (4)	0.0051 (4)	0.0019 (4)
C10	0.0291 (6)	0.0291 (6)	0.0193 (5)	−0.0039 (5)	0.0033 (5)	−0.0025 (4)
C11	0.0226 (5)	0.0211 (5)	0.0160 (5)	−0.0011 (4)	0.0060 (4)	0.0000 (4)
C12	0.0229 (6)	0.0250 (6)	0.0210 (5)	0.0011 (4)	0.0048 (4)	0.0008 (4)
C13	0.0215 (5)	0.0247 (6)	0.0252 (5)	0.0000 (4)	0.0073 (4)	−0.0018 (4)
C14	0.0231 (6)	0.0401 (7)	0.0365 (7)	0.0047 (5)	0.0117 (5)	0.0007 (6)
C15	0.0207 (5)	0.0202 (5)	0.0204 (5)	−0.0025 (4)	0.0056 (4)	0.0022 (4)
C16	0.0282 (6)	0.0228 (5)	0.0209 (5)	−0.0051 (4)	0.0071 (5)	0.0005 (4)
C17	0.0336 (7)	0.0282 (6)	0.0236 (6)	−0.0082 (5)	0.0000 (5)	0.0055 (5)
C18	0.0277 (6)	0.0300 (6)	0.0367 (7)	−0.0001 (5)	−0.0004 (5)	0.0090 (5)
C19	0.0287 (6)	0.0302 (6)	0.0368 (7)	0.0056 (5)	0.0086 (5)	0.0034 (5)
C20	0.0266 (6)	0.0268 (6)	0.0239 (6)	0.0031 (4)	0.0079 (5)	0.0013 (4)

Geometric parameters (Å, º)

O1—C7	1.2482 (13)	C8—C11	1.4611 (14)
N1—N2	1.3842 (12)	C9—C10	1.4862 (16)
N1—C7	1.3894 (13)	C10—H10A	0.94 (2)
N1—C1	1.4165 (14)	C10—H10B	0.98 (2)
N2—C9	1.3498 (14)	C10—H10C	0.98 (2)
N2—H2A	0.948 (17)	C11—C12	1.3813 (16)
N3—C13	1.3289 (15)	C12—C13	1.4102 (15)
N3—N4	1.3686 (12)	C12—H12	0.995 (16)

N4—C11	1.3723 (13)	C13—C14	1.4961 (16)
N4—C15	1.4204 (14)	C14—H14A	1.03 (2)
C1—C6	1.3920 (17)	C14—H14B	0.99 (2)
C1—C2	1.3939 (15)	C14—H14C	1.006 (18)
C2—C3	1.3890 (18)	C15—C16	1.3892 (15)
C2—H2	0.991 (16)	C15—C20	1.3897 (15)
C3—C4	1.381 (2)	C16—C17	1.3871 (17)
C3—H3	1.036 (19)	C16—H16	0.965 (15)
C4—C5	1.386 (2)	C17—C18	1.3848 (19)
C4—H4	0.977 (18)	C17—H17	1.000 (16)
C5—C6	1.3887 (17)	C18—C19	1.3845 (19)
C5—H5	0.997 (17)	C18—H18	1.001 (17)
C6—H6	0.976 (16)	C19—C20	1.3899 (18)
C7—C8	1.4359 (15)	C19—H19	0.983 (18)
C8—C9	1.3777 (14)	C20—H20	0.975 (15)

N2—N1—C7	109.19 (9)	C9—C10—H10B	110.0 (13)
N2—N1—C1	120.38 (8)	H10A—C10—H10B	104.2 (18)
C7—N1—C1	130.15 (9)	C9—C10—H10C	112.2 (13)
C9—N2—N1	108.47 (8)	H10A—C10—H10C	110.2 (18)
C9—N2—H2A	123.6 (10)	H10B—C10—H10C	107.3 (18)
N1—N2—H2A	120.0 (10)	N4—C11—C12	105.95 (9)
C13—N3—N4	104.96 (9)	N4—C11—C8	123.62 (10)
N3—N4—C11	111.94 (9)	C12—C11—C8	130.31 (10)
N3—N4—C15	118.33 (8)	C11—C12—C13	105.67 (10)
C11—N4—C15	129.72 (9)	C11—C12—H12	127.6 (9)
C6—C1—C2	120.03 (11)	C13—C12—H12	126.7 (9)
C6—C1—N1	120.32 (10)	N3—C13—C12	111.47 (10)
C2—C1—N1	119.64 (10)	N3—C13—C14	119.70 (10)
C3—C2—C1	119.49 (12)	C12—C13—C14	128.81 (11)
C3—C2—H2	121.3 (9)	C13—C14—H14A	110.9 (12)
C1—C2—H2	119.2 (9)	C13—C14—H14B	110.9 (13)
C4—C3—C2	120.90 (12)	H14A—C14—H14B	106.5 (17)
C4—C3—H3	120.0 (10)	C13—C14—H14C	110.9 (10)
C2—C3—H3	119.1 (10)	H14A—C14—H14C	108.7 (15)
C3—C4—C5	119.22 (12)	H14B—C14—H14C	108.8 (15)
C3—C4—H4	121.7 (10)	C16—C15—C20	120.51 (11)
C5—C4—H4	119.1 (10)	C16—C15—N4	118.80 (10)
C4—C5—C6	120.97 (13)	C20—C15—N4	120.66 (10)
C4—C5—H5	120.3 (10)	C17—C16—C15	119.23 (11)
C6—C5—H5	118.7 (10)	C17—C16—H16	121.3 (8)
C5—C6—C1	119.38 (11)	C15—C16—H16	119.4 (8)
C5—C6—H6	121.2 (9)	C18—C17—C16	120.84 (11)
C1—C6—H6	119.4 (9)	C18—C17—H17	120.0 (9)
O1—C7—N1	123.78 (10)	C16—C17—H17	119.2 (9)
O1—C7—C8	130.87 (10)	C19—C18—C17	119.44 (12)
N1—C7—C8	105.35 (9)	C19—C18—H18	119.7 (10)
C9—C8—C7	107.50 (9)	C17—C18—H18	120.9 (10)

C9—C8—C11	127.39 (10)	C18—C19—C20	120.58 (12)
C7—C8—C11	124.98 (9)	C18—C19—H19	120.0 (10)
N2—C9—C8	109.39 (9)	C20—C19—H19	119.4 (10)
N2—C9—C10	119.95 (9)	C15—C20—C19	119.35 (11)
C8—C9—C10	130.65 (10)	C15—C20—H20	119.3 (9)
C9—C10—H10A	112.6 (14)	C19—C20—H20	121.3 (9)
C7—N1—N2—C9	−2.24 (12)	C7—C8—C9—C10	178.44 (11)
C1—N1—N2—C9	−176.77 (9)	C11—C8—C9—C10	2.4 (2)
C13—N3—N4—C11	−0.78 (12)	N3—N4—C11—C12	0.82 (12)
C13—N3—N4—C15	177.91 (9)	C15—N4—C11—C12	−177.69 (10)
N2—N1—C1—C6	−166.17 (10)	N3—N4—C11—C8	−175.64 (10)
C7—N1—C1—C6	20.60 (18)	C15—N4—C11—C8	5.86 (17)
N2—N1—C1—C2	12.62 (15)	C9—C8—C11—N4	−128.38 (12)
C7—N1—C1—C2	−160.61 (11)	C7—C8—C11—N4	56.22 (16)
C6—C1—C2—C3	1.15 (19)	C9—C8—C11—C12	56.09 (18)
N1—C1—C2—C3	−177.64 (11)	C7—C8—C11—C12	−119.31 (14)
C1—C2—C3—C4	−0.5 (2)	N4—C11—C12—C13	−0.51 (12)
C2—C3—C4—C5	−0.3 (2)	C8—C11—C12—C13	175.62 (11)
C3—C4—C5—C6	0.6 (2)	N4—N3—C13—C12	0.43 (13)
C4—C5—C6—C1	0.0 (2)	N4—N3—C13—C14	178.99 (10)
C2—C1—C6—C5	−0.85 (18)	C11—C12—C13—N3	0.05 (13)
N1—C1—C6—C5	177.93 (11)	C11—C12—C13—C14	−178.34 (12)
N2—N1—C7—O1	−179.69 (10)	N3—N4—C15—C16	39.09 (14)
C1—N1—C7—O1	−5.87 (19)	C11—N4—C15—C16	−142.49 (11)
N2—N1—C7—C8	0.41 (12)	N3—N4—C15—C20	−139.05 (11)
C1—N1—C7—C8	174.23 (10)	C11—N4—C15—C20	39.37 (16)
O1—C7—C8—C9	−178.38 (12)	C20—C15—C16—C17	−2.36 (16)
N1—C7—C8—C9	1.52 (12)	N4—C15—C16—C17	179.50 (10)
O1—C7—C8—C11	−2.21 (19)	C15—C16—C17—C18	1.51 (17)
N1—C7—C8—C11	177.68 (10)	C16—C17—C18—C19	0.29 (18)
N1—N2—C9—C8	3.23 (12)	C17—C18—C19—C20	−1.27 (19)
N1—N2—C9—C10	−177.99 (9)	C16—C15—C20—C19	1.40 (17)
C7—C8—C9—N2	−2.95 (12)	N4—C15—C20—C19	179.50 (11)
C11—C8—C9—N2	−179.00 (10)	C18—C19—C20—C15	0.44 (19)

Hydrogen-bond geometry (Å, º)

Cg2, Cg3 and Cg4 are the centroids of the N3/N4/C11–C13, C1–C6 and C15–C20 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.948 (17)	1.788 (17)	2.7326 (12)	173.8 (15)
C2—H2···O1^{i}	0.991 (16)	2.490 (16)	3.2058 (15)	128.8 (12)
C6—H6···O1	0.976 (16)	2.282 (16)	2.9210 (15)	122.2 (12)
C5—H5···*Cg*3^{ii}	0.997 (17)	2.706 (16)	3.6201 (15)	153.0 (12)
C10—H10*A*···*Cg*2^{iii}	0.94 (2)	2.79 (2)	3.5373 (13)	136.5 (18)

C10—H10*B*···*Cg*4^{iv}	0.98 (2)	2.83 (2)	3.7117 (14)	150.3 (17)
C14—H14*B*···*Cg*2^{v}	0.99 (2)	2.77 (2)	3.6861 (16)	154.9 (16)

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $-x$, $y-1/2$, $-z+3/2$; (iii) x, $-y-1/2$, $z-1/2$; (iv) x, $-y+1/2$, $z-1/2$; (v) $-x+1$, $y-1/2$, $-z+3/2$.