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

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

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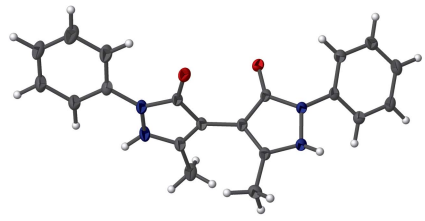
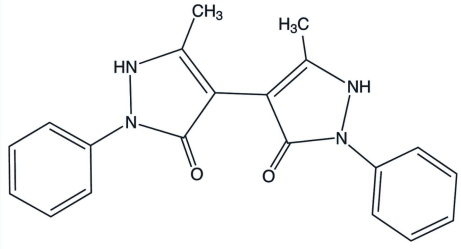
The title compound, $C_{20}H_{18}N_4O_2$, known as bispyrazolone, was crystallized from dimethyl sulfoxide. The structure has orthorhombic (*Pbca*) symmetry at 150 K, and displays both intra- and intermolecular hydrogen bonding through C—H···O and N—H···O contacts, respectively. None of the phenyl and pyrazolone rings in the molecule are coplanar. The dihedral angle between the pyrazolone rings is 66.18 (5)°.

3D view



Chemical scheme



Structure description

Pyrazolones have been studied as antipyretics and analgesics (Brune, 1997; Badawey & El–Ashmawey, 1998; Gürsoy *et al.*, 2000), as anxiolytics (Geronikaki *et al.*, 2004), and as antihyperglycemic agents (Kees *et al.*, 1996). These compound types have also been found to have antioxidant and neuroprotective activities, and have been used to treat amyotrophic lateral sclerosis (ALS) and ischemia (Watanabe *et al.*, 2004; Yoshida *et al.*, 2006; Yuan *et al.*, 2008). Pyrazolones have also been looked at as potential HIV-1 integrase inhibitors (Hadi, *et al.*, 2010). In addition to the multitude of possibilities in medicinal chemistry, pyrazolone research has led to prospective antimicrobial compounds (Chande *et al.*, 2007) and corrosion inhibitors (Elmorsi & Hassanein, 1999). The title compound, bispyrazolone, is primarily used as part of a pyridine-pyrazolone reagent for the detection of amine compounds. This method can quantify levels of cyanide (Epstein, 1947), ammonia and cyanate (Kruse & Mellon, 1952), and urea (Sharma *et al.*, 2013). It may also be used to determine the percentage of nitrogen in steel samples (Lear & Mellon, 1957). Bispyrazolone and similar derivatives have also been examined as color developers (Bavley, 1946) and as lubricating oil thickeners (McGrath and Pellegrini, 1961) for high-temperature greases.

In the crystal structure of the title compound, the molecules are non-planar (Fig. 1). The dihedral angle between the two pyrazolone rings is 66.18 (5)°, while that between the

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.89 (2)	1.85 (2)	2.7313 (14)	175.1 (18)
N4—H4···O1^{ii}	0.93 (2)	1.81 (2)	2.7321 (15)	169.3 (18)
C20—H20···O2	0.95 (2)	2.23 (2)	2.8988 (17)	126.5 (16)

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

phenyl rings is 39.44 (6)°. The ring systems in the halves of the molecules have significantly different degrees of rotation with respect to one another. The dihedral angle between the C9–C14 phenyl ring and the N1/N2/C1–C3 pyrazolone ring is 34.29 (6)° while that between the C15–C20 phenyl ring and the N3/N4/C5–C7 pyrazolone ring is 13.75 (7)°. The latter is a consequence of intramolecular C—H···O hydrogen bonding between the C20—H20 group on the phenyl ring and the O2 atom of the pyrazolone ring (Table 1, Fig. 2).

In the crystal, the molecules pack in a manner that maximizes intermolecular hydrogen bonding. Both oxygen atoms and both N—H groups of each bispyrazolone molecule are involved in forming four hydrogen bonds with three neighboring molecules (Table 1, Fig. 2). The intermolecular hydrogen bond axes lie approximately in the *bc* plane of the unit cell. Thus hydrogen-bonded sheets of the molecules stack perpendicular to the *a* axis (Fig. 3).

Synthesis and crystallization

A sample of the title compound was used as received from Sigma–Aldrich, and dissolved in hot dimethylsulfoxide. Colorless crystals were obtained by slow cooling of this solution to 298 K.

Refinement

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

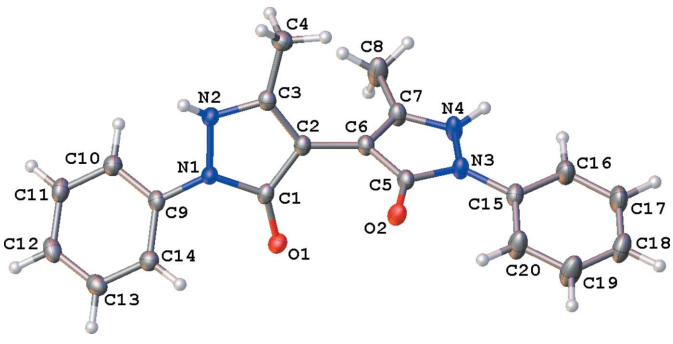


Figure 1
The title molecule with the labeling scheme and displacement ellipsoids drawn at the 50% probability level.

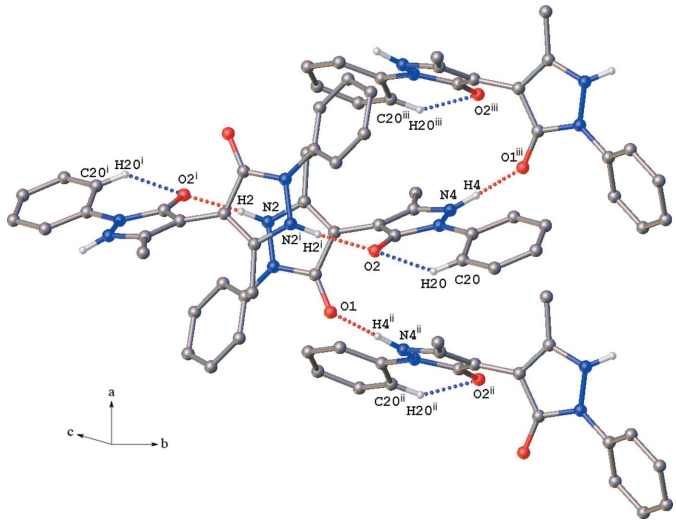


Figure 2
View of the intramolecular (blue dotted lines) and intermolecular (red dotted lines) hydrogen bond interactions. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $-\frac{1}{2}+x, \frac{3}{2}-y, 1-z$; (iii) $\frac{1}{2}+x, \frac{3}{2}-y, 1-z$.]

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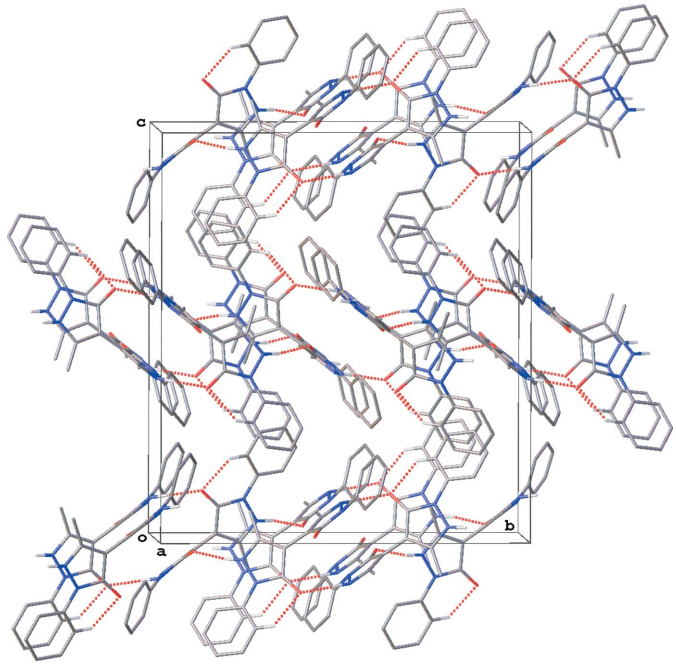

Figure 3
Packing of the molecules viewed approximately along the *a* axis with hydrogen bonds shown as dotted lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{18}N_4O_2$
M_r	346.38
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	150
a, *b*, *c* (Å)	8.7438 (1), 18.7561 (2), 20.8005 (2)
V (Å^3)	3411.27 (6)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	0.73
Crystal size (mm)	0.27 × 0.21 × 0.03
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Cu, AtlasS2 CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)
T_{min}, T_{max}	0.874, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16964, 3336, 3020
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.113, 1.04
No. of reflections	3336
No. of parameters	307
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.25

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

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Crystal data

$C_{20}H_{18}N_4O_2$
M_r = 346.38
Orthorhombic, *Pbca*
a = 8.7438 (1) Å
b = 18.7561 (2) Å
c = 20.8005 (2) Å
V = 3411.27 (6) Å^3
Z = 8
F(000) = 1456
D_x = 1.349 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 9599 reflections
θ = 4.7–72.3°
μ = 0.73 mm^{-1}
T = 150 K
Plate, clear colourless
0.27 × 0.21 × 0.03 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Cu, AtlasS2 CCD diffractometer
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.2387 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)
T_{min} = 0.874, T_{max} = 1.000
16964 measured reflections
3336 independent reflections
3020 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 72.6°, θ_{min} = 4.3°
h = −7→10
k = −22→23
l = −25→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 1.04
3336 reflections
307 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 1.0751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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. The H atoms bound to N2 and N4 were located in a difference map and refined. All hydrogen atoms were located in a difference map and were refined isotropically without constraints.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.17850 (10)	0.59409 (5)	0.52406 (4)	0.0228 (2)
O2	0.41464 (11)	0.62429 (5)	0.38211 (4)	0.0254 (2)
N1	0.33303 (11)	0.51616 (5)	0.58208 (5)	0.0197 (2)
N2	0.48738 (12)	0.51224 (6)	0.59817 (5)	0.0203 (2)
H2	0.525 (2)	0.4688 (11)	0.6043 (9)	0.040 (5)*
N3	0.49474 (13)	0.74084 (6)	0.40463 (5)	0.0228 (2)
N4	0.53811 (15)	0.77703 (6)	0.45972 (6)	0.0283 (3)
H4	0.587 (2)	0.8209 (12)	0.4598 (9)	0.043 (5)*
C1	0.30864 (14)	0.57394 (6)	0.54173 (6)	0.0189 (3)
C2	0.45779 (14)	0.60260 (6)	0.52877 (6)	0.0200 (3)
C3	0.56144 (15)	0.56250 (6)	0.56271 (6)	0.0205 (3)
C4	0.73088 (16)	0.56807 (8)	0.56622 (7)	0.0280 (3)
H4A	0.760 (2)	0.5841 (11)	0.6082 (10)	0.047 (5)*
H4B	0.769 (2)	0.6027 (12)	0.5330 (10)	0.048 (5)*
H4C	0.781 (2)	0.5205 (13)	0.5591 (11)	0.057 (6)*
C5	0.46008 (14)	0.67053 (6)	0.42150 (6)	0.0206 (3)
C6	0.48650 (14)	0.66557 (6)	0.48898 (6)	0.0210 (3)
C7	0.53634 (16)	0.73124 (7)	0.50942 (7)	0.0252 (3)
C8	0.5806 (2)	0.75544 (8)	0.57491 (7)	0.0378 (4)
H8A	0.615 (3)	0.7180 (16)	0.6015 (14)	0.088 (9)*
H8B	0.657 (3)	0.7932 (13)	0.5731 (11)	0.060 (6)*
H8C	0.490 (3)	0.7748 (16)	0.5982 (14)	0.086 (9)*
C9	0.22459 (14)	0.47963 (6)	0.62063 (6)	0.0203 (3)
C10	0.26090 (16)	0.46291 (7)	0.68395 (7)	0.0249 (3)
H10	0.3582 (19)	0.4766 (9)	0.7016 (8)	0.028 (4)*
C11	0.15554 (16)	0.42644 (7)	0.72142 (7)	0.0282 (3)
H11	0.1800 (19)	0.4165 (9)	0.7650 (9)	0.030 (4)*
C12	0.01470 (16)	0.40714 (7)	0.69603 (7)	0.0280 (3)
H12	−0.060 (2)	0.3814 (9)	0.7228 (9)	0.033 (4)*
C13	−0.02218 (15)	0.42573 (7)	0.63351 (7)	0.0264 (3)
H13	−0.122 (2)	0.4129 (9)	0.6151 (8)	0.031 (4)*
C14	0.08272 (15)	0.46155 (7)	0.59499 (7)	0.0234 (3)
H14	0.0610 (18)	0.4727 (9)	0.5502 (8)	0.025 (4)*
C15	0.47280 (15)	0.77740 (7)	0.34550 (6)	0.0232 (3)
C16	0.52997 (19)	0.84583 (8)	0.33728 (8)	0.0349 (4)
H16	0.585 (2)	0.8683 (12)	0.3736 (11)	0.056 (6)*
C17	0.5073 (2)	0.88090 (8)	0.27926 (8)	0.0388 (4)
H17	0.552 (2)	0.9301 (11)	0.2736 (10)	0.046 (5)*
C18	0.4295 (2)	0.84888 (8)	0.22973 (7)	0.0368 (4)
H18	0.417 (2)	0.8738 (10)	0.1885 (9)	0.040 (5)*
C19	0.3694 (2)	0.78142 (9)	0.23859 (8)	0.0440 (4)
H19	0.313 (2)	0.7578 (12)	0.2045 (11)	0.054 (6)*
C20	0.3906 (2)	0.74557 (8)	0.29632 (7)	0.0367 (4)
H20	0.352 (2)	0.6986 (12)	0.3029 (10)	0.051 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0240 (5)	0.0187 (4)	0.0256 (5)	0.0027 (3)	−0.0025 (4)	0.0029 (3)
O2	0.0357 (5)	0.0157 (4)	0.0249 (5)	−0.0017 (3)	−0.0066 (4)	0.0006 (3)
N1	0.0195 (5)	0.0171 (5)	0.0225 (5)	0.0002 (4)	−0.0011 (4)	0.0039 (4)
N2	0.0209 (5)	0.0164 (5)	0.0236 (6)	0.0011 (4)	−0.0016 (4)	0.0029 (4)
N3	0.0324 (6)	0.0162 (5)	0.0197 (5)	−0.0033 (4)	−0.0008 (4)	0.0012 (4)
N4	0.0449 (7)	0.0185 (5)	0.0213 (6)	−0.0102 (5)	−0.0016 (5)	0.0012 (4)
C1	0.0256 (6)	0.0143 (5)	0.0167 (6)	0.0014 (4)	−0.0002 (5)	0.0000 (4)
C2	0.0255 (6)	0.0156 (6)	0.0190 (6)	−0.0012 (4)	−0.0001 (5)	0.0005 (5)
C3	0.0248 (6)	0.0167 (5)	0.0200 (6)	−0.0008 (5)	0.0007 (5)	−0.0007 (5)
C4	0.0241 (7)	0.0275 (7)	0.0324 (8)	−0.0017 (5)	−0.0014 (6)	0.0024 (6)
C5	0.0231 (6)	0.0147 (5)	0.0241 (6)	0.0002 (4)	0.0000 (5)	0.0022 (5)
C6	0.0246 (6)	0.0166 (6)	0.0219 (6)	−0.0014 (5)	0.0006 (5)	0.0018 (5)
C7	0.0339 (7)	0.0193 (6)	0.0224 (7)	−0.0040 (5)	0.0005 (5)	0.0014 (5)
C8	0.0647 (11)	0.0249 (7)	0.0238 (7)	−0.0129 (7)	−0.0052 (7)	−0.0002 (6)
C9	0.0236 (6)	0.0141 (5)	0.0233 (6)	0.0005 (4)	0.0021 (5)	0.0019 (4)
C10	0.0266 (6)	0.0227 (6)	0.0255 (7)	−0.0013 (5)	−0.0012 (5)	0.0033 (5)
C11	0.0332 (7)	0.0262 (6)	0.0253 (7)	0.0020 (5)	0.0031 (6)	0.0079 (5)
C12	0.0275 (7)	0.0216 (6)	0.0350 (8)	0.0008 (5)	0.0096 (6)	0.0051 (5)
C13	0.0229 (6)	0.0206 (6)	0.0357 (8)	−0.0004 (5)	0.0013 (6)	0.0010 (5)
C14	0.0245 (6)	0.0198 (6)	0.0258 (7)	0.0009 (5)	−0.0009 (5)	0.0012 (5)
C15	0.0285 (6)	0.0192 (6)	0.0218 (6)	0.0020 (5)	0.0035 (5)	0.0035 (5)
C16	0.0443 (8)	0.0274 (7)	0.0330 (8)	−0.0110 (6)	−0.0079 (7)	0.0083 (6)
C17	0.0509 (9)	0.0276 (7)	0.0381 (9)	−0.0095 (6)	−0.0046 (7)	0.0127 (6)
C18	0.0549 (9)	0.0295 (7)	0.0261 (7)	0.0019 (7)	−0.0006 (7)	0.0088 (6)
C19	0.0753 (12)	0.0302 (7)	0.0265 (8)	−0.0055 (8)	−0.0128 (8)	0.0028 (6)
C20	0.0616 (10)	0.0210 (7)	0.0274 (8)	−0.0076 (7)	−0.0076 (7)	0.0029 (6)

Geometric parameters (Å, º)

O1—C1	1.2540 (15)	C8—H8C	1.00 (3)
O2—C5	1.2577 (16)	C9—C10	1.3908 (18)
N1—N2	1.3924 (15)	C9—C14	1.3922 (18)
N1—C1	1.3873 (15)	C10—H10	0.962 (17)
N1—C9	1.4182 (16)	C10—C11	1.3870 (19)
N2—H2	0.89 (2)	C11—H11	0.950 (18)
N2—C3	1.3608 (16)	C11—C12	1.388 (2)
N3—N4	1.3848 (15)	C12—H12	0.986 (18)
N3—C5	1.3979 (15)	C12—C13	1.384 (2)
N3—C15	1.4211 (16)	C13—H13	0.982 (18)
N4—H4	0.93 (2)	C13—C14	1.3908 (19)
N4—C7	1.3442 (17)	C14—H14	0.973 (17)
C1—C2	1.4361 (17)	C15—C16	1.3880 (19)
C2—C3	1.3732 (18)	C15—C20	1.385 (2)
C2—C6	1.4638 (17)	C16—H16	0.99 (2)
C3—C4	1.4870 (18)	C16—C17	1.389 (2)

C4—H4A	0.96 (2)	C17—H17	1.01 (2)
C4—H4B	1.01 (2)	C17—C18	1.373 (2)
C4—H4C	1.00 (2)	C18—H18	0.984 (19)
C5—C6	1.4255 (18)	C18—C19	1.382 (2)
C6—C7	1.3739 (18)	C19—H19	0.97 (2)
C7—C8	1.487 (2)	C19—C20	1.389 (2)
C8—H8A	0.94 (3)	C20—H20	0.95 (2)
C8—H8B	0.98 (2)		

N2—N1—C9	119.13 (10)	H8A—C8—H8B	110 (2)
C1—N1—N2	109.61 (10)	H8A—C8—H8C	104 (2)
C1—N1—C9	128.07 (10)	H8B—C8—H8C	108 (2)
N1—N2—H2	116.1 (12)	C10—C9—N1	119.46 (11)
C3—N2—N1	107.13 (10)	C10—C9—C14	120.74 (12)
C3—N2—H2	122.7 (12)	C14—C9—N1	119.80 (12)
N4—N3—C5	108.30 (10)	C9—C10—H10	120.3 (10)
N4—N3—C15	121.11 (10)	C11—C10—C9	119.46 (13)
C5—N3—C15	130.03 (11)	C11—C10—H10	120.3 (10)
N3—N4—H4	124.2 (12)	C10—C11—H11	118.9 (10)
C7—N4—N3	108.67 (11)	C10—C11—C12	120.27 (13)
C7—N4—H4	124.8 (12)	C12—C11—H11	120.8 (10)
O1—C1—N1	123.52 (11)	C11—C12—H12	120.1 (10)
O1—C1—C2	131.01 (11)	C13—C12—C11	119.90 (13)
N1—C1—C2	105.45 (10)	C13—C12—H12	120.0 (10)
C1—C2—C6	124.33 (11)	C12—C13—H13	120.7 (10)
C3—C2—C1	107.32 (11)	C12—C13—C14	120.61 (13)
C3—C2—C6	128.27 (12)	C14—C13—H13	118.7 (10)
N2—C3—C2	110.12 (11)	C9—C14—H14	119.2 (10)
N2—C3—C4	119.75 (11)	C13—C14—C9	118.99 (12)
C2—C3—C4	130.11 (12)	C13—C14—H14	121.7 (10)
C3—C4—H4A	109.2 (12)	C16—C15—N3	120.27 (13)
C3—C4—H4B	110.2 (12)	C20—C15—N3	120.08 (12)
C3—C4—H4C	111.4 (13)	C20—C15—C16	119.63 (13)
H4A—C4—H4B	109.6 (17)	C15—C16—H16	118.3 (13)
H4A—C4—H4C	107.4 (18)	C15—C16—C17	119.58 (14)
H4B—C4—H4C	109.1 (17)	C17—C16—H16	122.1 (13)
O2—C5—N3	123.75 (12)	C16—C17—H17	118.7 (11)
O2—C5—C6	130.37 (11)	C18—C17—C16	121.05 (14)
N3—C5—C6	105.88 (10)	C18—C17—H17	120.2 (11)
C5—C6—C2	125.56 (11)	C17—C18—H18	120.2 (11)
C7—C6—C2	127.07 (12)	C17—C18—C19	119.25 (14)
C7—C6—C5	107.31 (11)	C19—C18—H18	120.6 (11)
N4—C7—C6	109.78 (12)	C18—C19—H19	120.9 (13)
N4—C7—C8	120.43 (12)	C18—C19—C20	120.51 (15)
C6—C7—C8	129.77 (12)	C20—C19—H19	118.6 (13)
C7—C8—H8A	113.1 (18)	C15—C20—C19	119.94 (14)
C7—C8—H8B	111.4 (14)	C15—C20—H20	118.5 (13)
C7—C8—H8C	110.3 (16)	C19—C20—H20	121.5 (13)

O1—C1—C2—C3	176.71 (13)	C1—C2—C6—C7	110.02 (16)
O1—C1—C2—C6	−0.3 (2)	C2—C6—C7—N4	−175.33 (13)
O2—C5—C6—C2	−3.0 (2)	C2—C6—C7—C8	3.0 (3)
O2—C5—C6—C7	179.71 (14)	C3—C2—C6—C5	116.89 (15)
N1—N2—C3—C2	5.32 (14)	C3—C2—C6—C7	−66.4 (2)
N1—N2—C3—C4	−175.97 (11)	C5—N3—N4—C7	1.98 (15)
N1—C1—C2—C3	−1.56 (14)	C5—N3—C15—C16	−173.56 (14)
N1—C1—C2—C6	−178.61 (11)	C5—N3—C15—C20	8.1 (2)
N1—C9—C10—C11	−179.24 (12)	C5—C6—C7—N4	1.88 (16)
N1—C9—C14—C13	180.00 (11)	C5—C6—C7—C8	−179.78 (16)
N2—N1—C1—O1	−173.60 (11)	C6—C2—C3—N2	174.55 (12)
N2—N1—C1—C2	4.83 (13)	C6—C2—C3—C4	−4.0 (2)
N2—N1—C9—C10	23.01 (16)	C9—N1—N2—C3	−167.76 (11)
N2—N1—C9—C14	−157.62 (11)	C9—N1—C1—O1	−14.3 (2)
N3—N4—C7—C6	−2.41 (16)	C9—N1—C1—C2	164.12 (12)
N3—N4—C7—C8	179.07 (14)	C9—C10—C11—C12	−0.3 (2)
N3—C5—C6—C2	176.64 (12)	C10—C9—C14—C13	−0.64 (19)
N3—C5—C6—C7	−0.62 (14)	C10—C11—C12—C13	−1.4 (2)
N3—C15—C16—C17	−179.85 (14)	C11—C12—C13—C14	2.2 (2)
N3—C15—C20—C19	−179.98 (15)	C12—C13—C14—C9	−1.17 (19)
N4—N3—C5—O2	178.89 (12)	C14—C9—C10—C11	1.40 (19)
N4—N3—C5—C6	−0.81 (14)	C15—N3—N4—C7	174.20 (12)
N4—N3—C15—C16	16.11 (19)	C15—N3—C5—O2	7.6 (2)
N4—N3—C15—C20	−162.19 (14)	C15—N3—C5—C6	−172.10 (12)
C1—N1—N2—C3	−6.34 (13)	C15—C16—C17—C18	−0.2 (3)
C1—N1—C9—C10	−134.57 (13)	C16—C15—C20—C19	1.7 (3)
C1—N1—C9—C14	44.80 (18)	C16—C17—C18—C19	1.8 (3)
C1—C2—C3—N2	−2.35 (14)	C17—C18—C19—C20	−1.6 (3)
C1—C2—C3—C4	179.11 (13)	C18—C19—C20—C15	−0.1 (3)
C1—C2—C6—C5	−66.70 (18)	C20—C15—C16—C17	−1.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.89 (2)	1.85 (2)	2.7313 (14)	175.1 (18)
N4—H4···O1^{ii}	0.93 (2)	1.81 (2)	2.7321 (15)	169.3 (18)
C20—H20···O2	0.95 (2)	2.23 (2)	2.8988 (17)	126.5 (16)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, −*z*+1.