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N-{2-[2-(5-Methyl-1*H*-pyrazol-3-yl)acetamido]-phenyl}benzamide monohydrate

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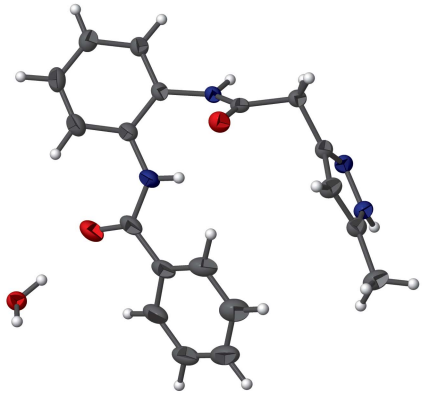
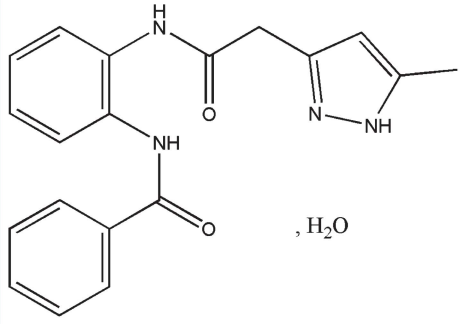
The asymmetric unit of the title compound, $C_{19}H_{18}N_4O_2\cdot H_2O$, comprises the U-shaped pyrazole derivative and a solvent water molecule. The molecular conformation is partly determined by an intramolecular N—H···O hydrogen bond. The crystal packing is directed by an extensive network of O—H···O, N—H···O, N—H···N and C—H···O hydrogen bonds together with C—H···π(ring) contacts that generate a three-dimensional network.

3D view



Chemical scheme



Structure description

Pyrazole derivatives have pharmacologically attractive biological applications (Havryluk *et al.*, 2016) and interesting therapeutic properties (Khan *et al.*, 2016). These compounds have been synthesized as target structures by many researchers and have been evaluated for their beneficial bioactivity and for the rational design of a new generation of small molecule drugs (Küçükgüzel & Şenkardeş, 2015). Continuing our research in this field (Chkirate *et al.*, 2001), we have synthesized *N*-2-benzamido-phenyl-5-methyl-pyrazol-3-yl acetamide by reacting benzoyl chloride with *N*-2-aminophenyl-5-methyl-pyrazol-3-yl acetamide. The latter was obtained by the action of hydrazine on the 4-(oxopropylidene)-1,5-benzodiazepin-2-one (El Abbassi *et al.*, 1989).

The title molecule adopts a U-shaped conformation due, in part, to the intramolecular N1—H1···O2 hydrogen bond (Table 1 and Fig. 1). The dihedral angle between the C1–C6 and C8–C13 benzene rings is 49.67 (5)° while that between the latter ring and the pyrazole ring is 64.49 (6)°. The packing is governed largely by a network of intermolecular hydrogen bonds including N2—H2*A*···N3^{i}, N4—H4*A*···O3^{ii}, O3—

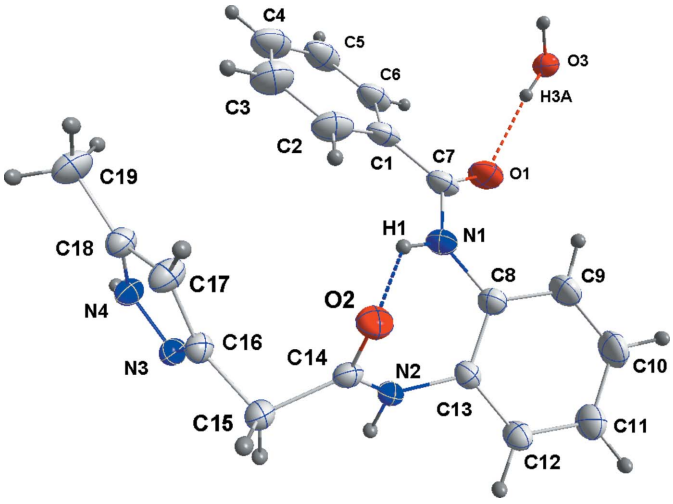


Figure 1
The asymmetric unit of the title compound, showing the atom-labelling scheme and 50% probability displacement ellipsoids. The intramolecular N—H···O hydrogen bond is shown as a blue dashed line.

H3*A*···O1, O3—H3*B*···O2^{iv} and C12—H12···O3^{iii} (Table 1 and Fig. 2). In addition there are two C—H···π(ring) interactions: C15—H15*A*···π(C8–C13)^{v} and C19—H19*A*···π(N3,N4,C16–C18)^{vi}, Table 1, that also contribute to the crystal packing. These contacts combine to generate a three-dimensional network, Fig. 2.

Synthesis and crystallization

To a solution of 5 × 10^{-4} mol of *N*-(2-aminophenyl-5-methyl-pyrazol-3-yl)acetamide dissolved in 10 ml of ethanol was added 5 × 10^{-4} mol of benzoyl chloride. The mixture was stirred for 24 h at room temperature. After filtration and recrystallization from ethanol, colourless single crystals were obtained with a yield of 66%.

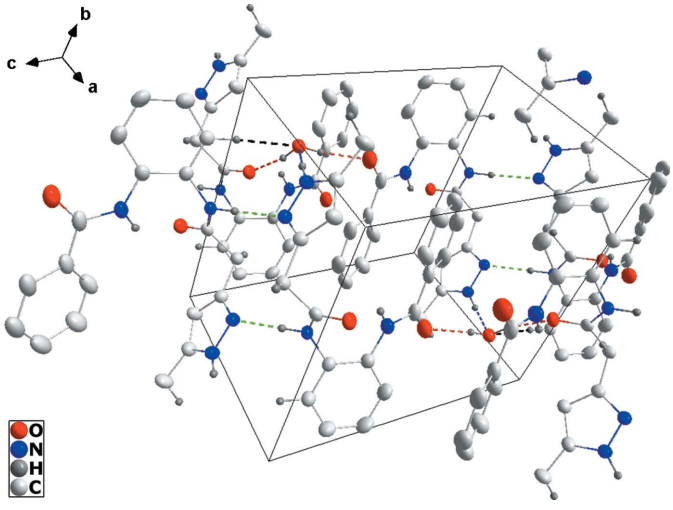


Figure 2
Crystal packing projected onto (111) with hydrogen bonds shown as dashed lines [O—H···O (red); N—H···O (blue); N—H···N (green); C—H···O (black)].

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

*Cg*1 and *Cg*3 are the centroids of the N3,N4,C16–C18 and C8–C13 rings respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.88 (2)	2.09 (2)	2.7902 (17)	135.0 (19)
N2—H2*A*···N3^{i}	0.95 (2)	1.98 (2)	2.9209 (17)	176.4 (17)
N4—H4*A*···O3^{ii}	0.92 (2)	1.88 (2)	2.7883 (16)	166.9 (19)
C12—H12···O3^{iii}	0.978 (19)	2.464 (19)	3.4042 (19)	161.2 (14)
O3—H3*A*···O1	0.87 (3)	1.89 (3)	2.7445 (16)	167 (2)
O3—H3*B*···O2^{iv}	0.94 (3)	1.83 (3)	2.7575 (15)	169 (2)
C15—H15*A*···*Cg*3^{v}	0.957 (19)	2.893 (18)	3.8485 (15)	174.0 (14)
C19—H19*A*···*Cg*1^{vi}	0.98 (3)	2.86 (3)	3.645 (2)	138 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{18}N_4O_2·H_2O$
M_r	352.39
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	8.4220 (3), 10.0410 (4), 10.8799 (4)
α, β, γ (°)	101.889 (2), 94.104 (2), 90.402 (1)
V (Å^3)	897.79 (6)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	0.74
Crystal size (mm)	0.15 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.85, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6831, 3279, 2846
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.114, 1.06
No. of reflections	3279
No. of parameters	316
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.21

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

Refinement

Crystal and refinement details appear in Table 2. Eleven reflections appearing near the top of the frames on which they were recorded were omitted from the fineal refinement as they appeared to have been partially obscured by the nozzle of the low-temperature attachment.

Acknowledgements

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full crystallographic data

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_N_-{2-[2-(5-Methyl-1_H_-pyrazol-3-yl)acetamido]phenyl}benzamide monohydrate

Crystal data

$C_{19}H_{18}N_4O_2·H_2O$
M_r = 352.39
Triclinic, $P\overline{1}$
a = 8.4220 (3) Å
b = 10.0410 (4) Å
c = 10.8799 (4) Å
α = 101.889 (2)°
β = 94.104 (2)°
γ = 90.402 (1)°
V = 897.79 (6) Å^3
Z = 2
F(000) = 372
D_x = 1.304 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 5496 reflections
θ = 4.5–71.9°
μ = 0.74 mm^{-1}
T = 150 K
Block, colourless
0.15 × 0.14 × 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} = 0.85, T_{max} = 0.93
6831 measured reflections
3279 independent reflections
2846 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 72.2°, θ_{min} = 4.2°
h = −10→10
k = −11→12
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.114
S = 1.06
3279 reflections
316 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
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.2007P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0164 (16)

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	0.79721 (16)	0.27601 (13)	0.44040 (10)	0.0459 (3)
O2	0.93031 (11)	0.56110 (10)	0.87382 (10)	0.0299 (3)
N1	0.83593 (16)	0.38781 (15)	0.64465 (12)	0.0344 (3)
H1	0.828 (3)	0.468 (2)	0.695 (2)	0.053 (6)*
N2	0.77023 (13)	0.38862 (11)	0.89936 (10)	0.0226 (3)
H2A	0.693 (2)	0.3631 (18)	0.9497 (18)	0.037 (5)*
N3	0.47391 (14)	0.69851 (11)	0.95462 (11)	0.0266 (3)
N4	0.42223 (14)	0.79751 (12)	0.89372 (11)	0.0275 (3)
H4A	0.315 (3)	0.798 (2)	0.870 (2)	0.050 (6)*
C1	0.73450 (18)	0.51188 (18)	0.48918 (14)	0.0354 (4)
C2	0.7643 (2)	0.63951 (19)	0.56712 (16)	0.0421 (4)
H2	0.830 (2)	0.651 (2)	0.648 (2)	0.050 (5)*
C3	0.7021 (2)	0.7553 (2)	0.53373 (19)	0.0514 (5)
H3	0.725 (3)	0.844 (3)	0.588 (2)	0.067 (7)*
C4	0.6082 (2)	0.7447 (2)	0.42178 (19)	0.0541 (5)
H4	0.569 (3)	0.827 (2)	0.402 (2)	0.062 (6)*
C5	0.5786 (2)	0.6188 (2)	0.34362 (17)	0.0499 (5)
H5	0.509 (3)	0.608 (2)	0.264 (2)	0.055 (6)*
C6	0.6409 (2)	0.5025 (2)	0.37623 (15)	0.0433 (4)
H6	0.619 (3)	0.408 (2)	0.321 (2)	0.055 (6)*
C7	0.79287 (18)	0.38224 (17)	0.52099 (14)	0.0352 (4)
C8	0.88775 (17)	0.27928 (15)	0.70092 (13)	0.0308 (3)
C9	0.9735 (2)	0.17147 (18)	0.63698 (16)	0.0416 (4)
H9	0.996 (3)	0.177 (2)	0.552 (2)	0.057 (6)*
C10	1.0224 (2)	0.06677 (18)	0.69444 (16)	0.0411 (4)
H10	1.082 (2)	−0.006 (2)	0.646 (2)	0.051 (6)*
C11	0.98655 (19)	0.06710 (15)	0.81653 (15)	0.0348 (3)
H11	1.020 (2)	−0.006 (2)	0.858 (2)	0.050 (6)*
C12	0.90333 (17)	0.17445 (14)	0.88159 (14)	0.0280 (3)
H12	0.880 (2)	0.1783 (17)	0.9689 (18)	0.033 (4)*
C13	0.85463 (15)	0.28126 (13)	0.82543 (13)	0.0247 (3)
C14	0.82037 (15)	0.51951 (13)	0.92651 (12)	0.0230 (3)
C15	0.73064 (17)	0.61472 (13)	1.02316 (13)	0.0254 (3)
H15A	0.810 (2)	0.6650 (18)	1.0828 (18)	0.035 (4)*
H15B	0.664 (2)	0.5616 (18)	1.0653 (17)	0.032 (4)*

C16	0.63237 (16)	0.71090 (13)	0.96200 (13)	0.0251 (3)
C17	0.68045 (17)	0.81614 (14)	0.90528 (15)	0.0305 (3)
H17	0.793 (2)	0.8410 (19)	0.8959 (18)	0.039 (5)*
C18	0.54213 (17)	0.86907 (14)	0.86181 (14)	0.0279 (3)
C19	0.5098 (2)	0.98073 (17)	0.79240 (18)	0.0390 (4)
H19A	0.445 (3)	1.052 (3)	0.838 (3)	0.079 (8)*
H19B	0.609 (3)	1.019 (2)	0.772 (2)	0.064 (7)*
H19C	0.445 (3)	0.947 (2)	0.714 (2)	0.052 (6)*
O3	0.89511 (12)	0.24005 (10)	0.20075 (10)	0.0295 (3)
H3A	0.872 (3)	0.263 (3)	0.278 (3)	0.074 (8)*
H3B	0.946 (3)	0.315 (3)	0.181 (2)	0.061 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0582 (7)	0.0541 (7)	0.0246 (6)	0.0020 (6)	0.0032 (5)	0.0061 (5)
O2	0.0293 (5)	0.0313 (5)	0.0310 (5)	−0.0026 (4)	0.0063 (4)	0.0097 (4)
N1	0.0403 (7)	0.0429 (7)	0.0214 (6)	0.0066 (6)	0.0041 (5)	0.0091 (5)
N2	0.0248 (5)	0.0240 (5)	0.0202 (5)	0.0007 (4)	0.0042 (4)	0.0061 (4)
N3	0.0275 (6)	0.0259 (6)	0.0275 (6)	0.0019 (4)	0.0033 (5)	0.0074 (4)
N4	0.0265 (6)	0.0270 (6)	0.0303 (6)	0.0021 (5)	0.0022 (5)	0.0090 (5)
C1	0.0303 (7)	0.0556 (10)	0.0240 (7)	−0.0008 (7)	0.0050 (6)	0.0156 (6)
C2	0.0413 (9)	0.0539 (10)	0.0349 (9)	−0.0047 (7)	−0.0044 (7)	0.0203 (7)
C3	0.0563 (11)	0.0548 (11)	0.0477 (11)	−0.0014 (9)	0.0004 (9)	0.0228 (9)
C4	0.0508 (11)	0.0746 (14)	0.0483 (11)	0.0143 (10)	0.0088 (9)	0.0368 (10)
C5	0.0385 (9)	0.0839 (14)	0.0327 (9)	0.0126 (9)	0.0027 (7)	0.0245 (9)
C6	0.0357 (8)	0.0713 (12)	0.0251 (8)	0.0046 (8)	0.0028 (6)	0.0151 (7)
C7	0.0323 (7)	0.0530 (9)	0.0217 (7)	−0.0005 (7)	0.0055 (6)	0.0099 (6)
C8	0.0311 (7)	0.0371 (8)	0.0245 (7)	0.0046 (6)	0.0032 (6)	0.0069 (6)
C9	0.0448 (9)	0.0514 (10)	0.0279 (8)	0.0117 (8)	0.0096 (7)	0.0041 (7)
C10	0.0412 (8)	0.0415 (9)	0.0370 (9)	0.0115 (7)	0.0082 (7)	−0.0023 (7)
C11	0.0359 (8)	0.0288 (7)	0.0389 (8)	0.0034 (6)	0.0042 (7)	0.0047 (6)
C12	0.0297 (7)	0.0266 (7)	0.0279 (7)	−0.0002 (5)	0.0041 (6)	0.0055 (5)
C13	0.0237 (6)	0.0267 (6)	0.0226 (7)	0.0000 (5)	0.0023 (5)	0.0026 (5)
C14	0.0241 (6)	0.0264 (6)	0.0200 (6)	0.0016 (5)	−0.0007 (5)	0.0089 (5)
C15	0.0297 (7)	0.0237 (6)	0.0234 (7)	0.0021 (5)	0.0023 (6)	0.0063 (5)
C16	0.0276 (6)	0.0218 (6)	0.0253 (7)	0.0007 (5)	0.0016 (5)	0.0036 (5)
C17	0.0275 (7)	0.0279 (7)	0.0386 (8)	−0.0009 (6)	0.0015 (6)	0.0128 (6)
C18	0.0307 (7)	0.0240 (6)	0.0297 (7)	−0.0011 (5)	0.0024 (6)	0.0071 (5)
C19	0.0421 (9)	0.0328 (8)	0.0464 (10)	0.0036 (7)	−0.0005 (8)	0.0191 (7)
O3	0.0316 (5)	0.0291 (5)	0.0289 (6)	−0.0006 (4)	0.0034 (4)	0.0082 (4)

Geometric parameters (Å, º)

O1—C7	1.236 (2)	C8—C9	1.397 (2)
O2—C14	1.2368 (16)	C8—C13	1.399 (2)
N1—C7	1.3578 (19)	C9—C10	1.380 (3)
N1—C8	1.413 (2)	C9—H9	0.97 (2)

N1—H1	0.88 (2)	C10—C11	1.382 (2)
N2—C14	1.3444 (17)	C10—H10	0.97 (2)
N2—C13	1.4316 (17)	C11—C12	1.386 (2)
N2—H2A	0.95 (2)	C11—H11	0.98 (2)
N3—C16	1.3346 (18)	C12—C13	1.390 (2)
N3—N4	1.3611 (16)	C12—H12	0.978 (19)
N4—C18	1.3414 (19)	C14—C15	1.5167 (18)
N4—H4A	0.92 (2)	C15—C16	1.5026 (19)
C1—C2	1.393 (3)	C15—H15A	0.957 (19)
C1—C6	1.398 (2)	C15—H15B	0.972 (19)
C1—C7	1.492 (2)	C16—C17	1.400 (2)
C2—C3	1.383 (3)	C17—C18	1.377 (2)
C2—H2	0.99 (2)	C17—H17	0.997 (19)
C3—C4	1.388 (3)	C18—C19	1.492 (2)
C3—H3	0.97 (3)	C19—H19A	0.98 (3)
C4—C5	1.380 (3)	C19—H19B	0.97 (3)
C4—H4	0.96 (2)	C19—H19C	0.98 (2)
C5—C6	1.385 (3)	O3—H3A	0.87 (3)
C5—H5	1.00 (2)	O3—H3B	0.94 (3)
C6—H6	1.02 (2)		

C7—N1—C8	127.23 (14)	C9—C10—C11	120.29 (14)
C7—N1—H1	115.9 (14)	C9—C10—H10	117.5 (13)
C8—N1—H1	116.9 (14)	C11—C10—H10	122.2 (13)
C14—N2—C13	123.60 (11)	C10—C11—C12	119.52 (15)
C14—N2—H2A	117.1 (11)	C10—C11—H11	121.3 (12)
C13—N2—H2A	117.0 (11)	C12—C11—H11	119.2 (12)
C16—N3—N4	104.44 (11)	C11—C12—C13	120.87 (14)
C18—N4—N3	112.75 (11)	C11—C12—H12	121.0 (10)
C18—N4—H4A	129.2 (13)	C13—C12—H12	118.1 (10)
N3—N4—H4A	117.3 (13)	C12—C13—C8	119.56 (13)
C2—C1—C6	118.94 (16)	C12—C13—N2	117.38 (12)
C2—C1—C7	123.71 (14)	C8—C13—N2	123.06 (13)
C6—C1—C7	117.33 (16)	O2—C14—N2	122.29 (12)
C3—C2—C1	120.71 (16)	O2—C14—C15	121.70 (12)
C3—C2—H2	117.6 (12)	N2—C14—C15	115.99 (12)
C1—C2—H2	121.7 (12)	C16—C15—C14	110.76 (11)
C2—C3—C4	119.9 (2)	C16—C15—H15A	109.7 (11)
C2—C3—H3	120.2 (15)	C14—C15—H15A	106.3 (11)
C4—C3—H3	119.9 (15)	C16—C15—H15B	110.7 (10)
C5—C4—C3	119.85 (19)	C14—C15—H15B	109.5 (10)
C5—C4—H4	123.0 (15)	H15A—C15—H15B	109.7 (15)
C3—C4—H4	117.1 (15)	N3—C16—C17	110.92 (12)
C4—C5—C6	120.57 (16)	N3—C16—C15	119.15 (12)
C4—C5—H5	121.4 (12)	C17—C16—C15	129.92 (13)
C6—C5—H5	118.0 (13)	C18—C17—C16	105.70 (13)
C5—C6—C1	120.03 (18)	C18—C17—H17	129.2 (11)
C5—C6—H6	121.8 (12)	C16—C17—H17	125.0 (11)

C1—C6—H6	118.1 (13)	N4—C18—C17	106.19 (12)
O1—C7—N1	122.37 (16)	N4—C18—C19	120.86 (13)
O1—C7—C1	122.02 (14)	C17—C18—C19	132.95 (14)
N1—C7—C1	115.58 (14)	C18—C19—H19A	112.3 (16)
C9—C8—C13	118.99 (14)	C18—C19—H19B	110.6 (14)
C9—C8—N1	122.09 (14)	H19A—C19—H19B	111 (2)
C13—C8—N1	118.91 (13)	C18—C19—H19C	110.7 (12)
C10—C9—C8	120.75 (15)	H19A—C19—H19C	104 (2)
C10—C9—H9	123.7 (13)	H19B—C19—H19C	108.2 (19)
C8—C9—H9	115.5 (13)	H3A—O3—H3B	107 (2)
C16—N3—N4—C18	0.84 (15)	C11—C12—C13—C8	1.1 (2)
C6—C1—C2—C3	0.1 (3)	C11—C12—C13—N2	−179.58 (13)
C7—C1—C2—C3	−177.84 (16)	C9—C8—C13—C12	−1.9 (2)
C1—C2—C3—C4	0.3 (3)	N1—C8—C13—C12	179.30 (13)
C2—C3—C4—C5	−0.6 (3)	C9—C8—C13—N2	178.78 (14)
C3—C4—C5—C6	0.4 (3)	N1—C8—C13—N2	0.0 (2)
C4—C5—C6—C1	0.1 (3)	C14—N2—C13—C12	120.82 (14)
C2—C1—C6—C5	−0.4 (2)	C14—N2—C13—C8	−59.84 (18)
C7—C1—C6—C5	177.75 (15)	C13—N2—C14—O2	11.49 (19)
C8—N1—C7—O1	−1.2 (3)	C13—N2—C14—C15	−170.30 (11)
C8—N1—C7—C1	176.82 (14)	O2—C14—C15—C16	68.48 (16)
C2—C1—C7—O1	−163.00 (17)	N2—C14—C15—C16	−109.73 (13)
C6—C1—C7—O1	19.0 (2)	N4—N3—C16—C17	−0.49 (15)
C2—C1—C7—N1	19.0 (2)	N4—N3—C16—C15	−179.14 (11)
C6—C1—C7—N1	−159.01 (14)	C14—C15—C16—N3	111.39 (14)
C7—N1—C8—C9	32.0 (2)	C14—C15—C16—C17	−66.96 (18)
C7—N1—C8—C13	−149.26 (15)	N3—C16—C17—C18	0.00 (16)
C13—C8—C9—C10	1.3 (3)	C15—C16—C17—C18	178.46 (13)
N1—C8—C9—C10	−179.91 (15)	N3—N4—C18—C17	−0.86 (16)
C8—C9—C10—C11	0.1 (3)	N3—N4—C18—C19	178.99 (13)
C9—C10—C11—C12	−1.0 (3)	C16—C17—C18—N4	0.50 (16)
C10—C11—C12—C13	0.4 (2)	C16—C17—C18—C19	−179.31 (16)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg3 are the centroids of the N3,N4,C16–C18 and C8–C13 rings respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.88 (2)	2.09 (2)	2.7902 (17)	135.0 (19)
N2—H2*A*···N3^{i}	0.95 (2)	1.98 (2)	2.9209 (17)	176.4 (17)
N4—H4*A*···O3^{ii}	0.92 (2)	1.88 (2)	2.7883 (16)	166.9 (19)
C12—H12···O3^{iii}	0.978 (19)	2.464 (19)	3.4042 (19)	161.2 (14)
O3—H3*A*···O1	0.87 (3)	1.89 (3)	2.7445 (16)	167 (2)
O3—H3*B*···O2^{iv}	0.94 (3)	1.83 (3)	2.7575 (15)	169 (2)
C15—H15*A*···*Cg*3^{v}	0.957 (19)	2.893 (18)	3.8485 (15)	174.0 (14)
C19—H19*A*···*Cg*1^{vi}	0.98 (3)	2.86 (3)	3.645 (2)	138 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*, *z*+1; (iv) −*x*+2, −*y*+1, −*z*+1; (v) −*x*+2, −*y*+1, −*z*+2; (vi) −*x*+1, −*y*+2, −*z*+2.