

# 5-Acetyl-6-methyl-4-phenyl-1-(prop-2-ynyl)-3,4-dihydropyrimidin-2(1H)-one

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Received 4 December 2017

Accepted 18 December 2017

Edited by C. Rizzoli, Università degli Studi di Parma, Italy

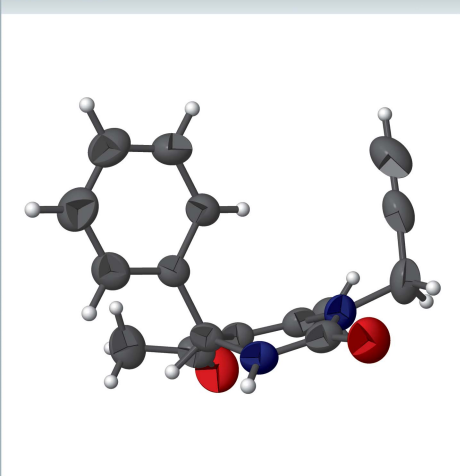
Keywords: crystal structure; acetyl; phenyl; 4-dihydropyrimidin-2(1H)-one; propynyl; hydrogen bonds.

CCDC reference: 1812012

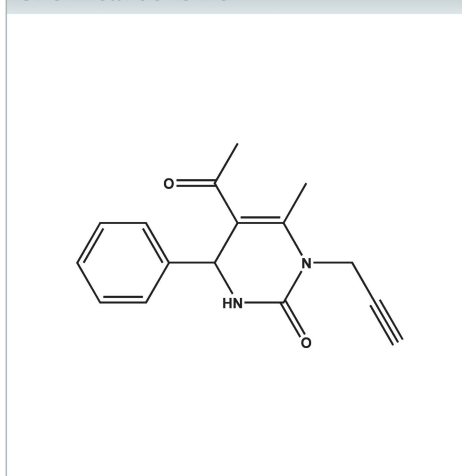
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

The 4-dihydropyrimidin-2(1H)-one moiety of the title molecule, C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>, displays a half-chair conformation. The least-squares mean plane through this heterocycle is almost perpendicular to the aromatic ring [dihedral angle = 89.52 (8)°] and to the prop-2-ynyl chain [C—C—N—C torsion angle of −73.2 (2)°]. The mean plane through the acetyl group makes a dihedral angle of 30.93 (10)° with the mean plane of the heterocycle. There is an intramolecular C—H···O hydrogen bond forming an S(6) ring motif. In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds forming inversion dimers.

## 3D view

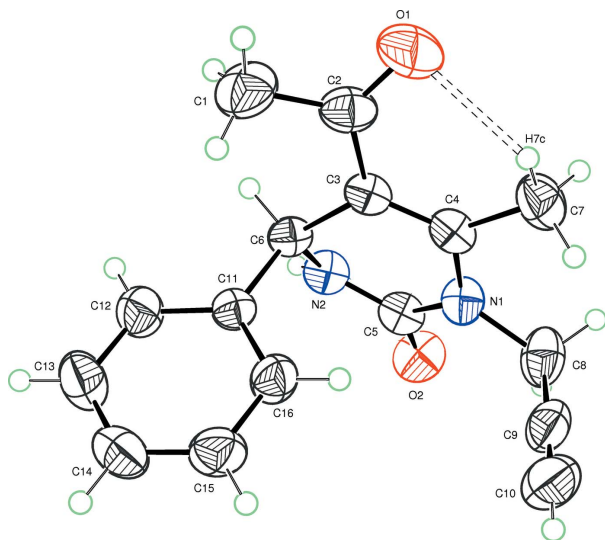


## Chemical scheme



## Structure description

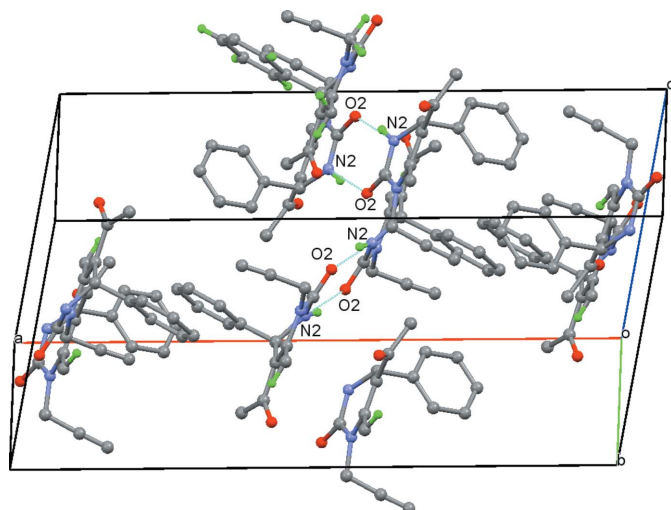
In past decades, dihydropyrimidinones (DHPMs) and their derivatives have attracted considerable interest due to their heterocyclic scaffold and interesting pharmacological properties such as antiviral, antitumor, anti-inflammatory as well their applications as calcium channel blockers and anticancer drugs (Ali *et al.*, 2016; Desai *et al.*, 2016; Xue *et al.*, 2016; Dalil *et al.*, 2016; Dhumaskar *et al.*, 2014; Jetli *et al.*, 2014). Different strategies have been used for the modification of 3,4-dihydropyrimidin-2(1H)-ones. For instance, *N*-alkylation is one of the most usable but other methods include mild base Cs<sub>2</sub>CO<sub>3</sub>, K<sub>2</sub>CO<sub>3</sub> (Putatunda *et al.*, 2012), the Mitsunobu-type reaction (Dallinger & Kappe, 2002), or phase-transfer catalysis (Singh *et al.*, 2009). Unfortunately, these strategies suffer from the disadvantage that the procedures need to be carried out in harsh conditions. In this



**Figure 1**  
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. The intramolecular hydrogen bond is shown as a dashed line.

article, we present a convenient approach for the preparation of an N1-alkylated DHPM derivative as a major product using potassium *t*-butoxide in DMF at room temperature.

The molecule of the title compound is built up from a 3,4-dihydropyrimidin-2(1*H*)-one ring linked to an acetyl group, one prop-2-ynyl chain and to methyl and phenyl groups as shown in Fig. 1. The dihydropyrimidine ring adopts a half-chair conformation as indicated by the total puckering amplitude  $Q_2 = 0.3602(15)$  Å, and spherical polar angle  $\theta = 106.8(2)^\circ$  with  $\varphi_2 = 10.5(2)^\circ$ . The dihedral angle between the mean plane passing through the heterocycle and that through the aromatic ring is  $89.52(8)^\circ$ . The prop-2-ynyl chain is nearly perpendicular to the mean plane of the dihydropyrimidine ring, as indicated by the C9–C8–N1–C4 torsion angle of  $-73.2(2)^\circ$ . The molecular conformation is stabilized by an



**Figure 2**  
Crystal packing of the title compound, showing molecules linked through N–H...O hydrogen bonds (dotted lines).

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

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C7–H7C...O1	0.96	2.21	2.862 (3)	125
N2–H2...O2 <sup>i</sup>	0.86	2.02	2.8612 (17)	164

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

intramolecular C–H...O hydrogen bond (Table 1), forming an *S*(6) ring motif. In the crystal, molecules are linked together by pairs of N–H...O hydrogen bonds, forming inversion dimers (Fig. 2, Table 1).

### Synthesis and crystallization

The title compound was prepared in good yield (70%) through condensation of 5-acetyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one (1 g, 4.34 mmol) with propargyl bromide (0.73 ml, 9.55 mmol) in the presence of potassium *t*-butoxide as a base in *N,N*-dimethylformamide (DMF, 10 ml) at room temperature for one h. After completion of the reaction (TLC), the product was extracted with ethyl acetate and washed with water ( $2 \times 20$  ml), the organic layer separated and dried over anhydrous sodium sulfate and the solvent was removed under reduced pressure. The resulting crude product was purified by a column packed with silica gel. The obtained product was crystallized by slow evaporation of *n*-hexane/ethyl acetate (7:3 v/v) mixture, m.p. 424 K.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
<i>M<sub>r</sub></i>	268.31
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	22.656 (2), 12.2607 (12), 10.2189 (10)
$\beta$ (°)	100.363 (4)
<i>V</i> (Å <sup>3</sup> )	2792.3 (5)
<i>Z</i>	8
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.09
Crystal size (mm)	0.36 × 0.28 × 0.22
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.645, 0.747
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	38459, 3614, 2502
<i>R<sub>int</sub></i>	0.047
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.676
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.046, 0.133, 1.02
No. of reflections	3614
No. of parameters	184
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.26, -0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

The confirmation of the synthesized compound was performed by spectroscopic techniques. The compound showed signals in its  $^1\text{H}$  NMR spectrum ( $\text{DMSO-}d_6$ )  $\delta = 2.09$  (*s*, 3H,  $\text{CH}_3\text{CO}$ ), 2.53 (*s*, 3H,  $\text{CH}_3$ ), 3.26 (*s*, 1H,  $\text{CH}$ ), 4.39–4.62 (*m*, 2H,  $-\text{CH}_2-$ ), 5.22 (*s*, 1H, H-4), 7.27–7.32 (*m*, 5H,  $\text{CAr}$ ), 8.13 (*s*, 1H,  $\text{N}_3-\text{H}$ ). The  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ ) spectrum signals appeared at:  $\delta = 196.06$  (CO), 151.92 (C-6), 147.32 (C-2), 142.99 (C-1'), 128.64 (C-4'), 128.64, 127.66 and 126.49 (other aromatic carbons), 113.23 (C-5), 80.31 (C-alkyne), 74.27 (CH-alkyne), 53.00 (C-4), 31.69 ( $-\text{CH}_2-$ ), 30.30 ( $\text{CH}_3$  at C-4'), 16.05 ( $\text{CH}_3$  at C-6). Further, ESI-MS  $[M + \text{H}]^+$  mass spectrum showed the  $[M+1]$  ion peak at  $m/z$  269.3, which is in agreement with the molecular formula  $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2$ . The IR spectrum of the compound showed an absorption band at 3301–3229  $\text{cm}^{-1}$  indicating the presence of  $\text{Csp-H}$  stretching. A strong absorption band at 3094  $\text{cm}^{-1}$  was attributed to the  $\text{N-H}$  stretching, and absorption bands at 2121, 1665, 1209  $\text{cm}^{-1}$  indicated the presence of  $\text{C}\equiv\text{C}$ ,  $\text{C}=\text{O}$  and  $\text{CN}$ . UV/Vis (MeOH):  $\lambda_{\text{max}} = 300$  and 222 nm.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Two outliers (200, 110) were omitted in the last cycles of refinement.

### Acknowledgements

The authors thank the Unit of Support for Technical and Scientific Research (UATRS, CNRST) for the X-ray measurements.

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## full crystallographic data

*IUCrData* (2017). **2**, x171802 [https://doi.org/10.1107/S2414314617018028]

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## 5-Acetyl-6-methyl-4-phenyl-1-(prop-2-ynyl)-3,4-dihydropyrimidin-2(1H)-one

*Crystal data*

$C_{16}H_{16}N_2O_2$

$M_r = 268.31$

Monoclinic,  $C2/c$

$a = 22.656$  (2) Å

$b = 12.2607$  (12) Å

$c = 10.2189$  (10) Å

$\beta = 100.363$  (4)°

$V = 2792.3$  (5) Å<sup>3</sup>

$Z = 8$

$F(000) = 1136$

$D_x = 1.276$  Mg m<sup>-3</sup>

Melting point: 424 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3614 reflections

$\theta = 2.7$ – $28.7^\circ$

$\mu = 0.09$  mm<sup>-1</sup>

$T = 296$  K

Prism, colourless

$0.36 \times 0.28 \times 0.22$  mm

*Data collection*

Bruker X8 APEX

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.645$ ,  $T_{\max} = 0.747$

38459 measured reflections

3614 independent reflections

2502 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 28.7^\circ$ ,  $\theta_{\min} = 2.7^\circ$

$h = -30 \rightarrow 30$

$k = -16 \rightarrow 16$

$l = -13 \rightarrow 11$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.133$

$S = 1.02$

3614 reflections

184 parameters

0 restraints

Hydrogen site location: inferred from

neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 1.4276P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

Extinction correction: SHELXL2014

(Sheldrick, 2015b),

$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0026 (5)

*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.** All H atoms were placed geometrically and isotropically refined with C–H = 0.93–0.98 Å, N–H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$  or  $1.5 U_{\text{eq}}(\text{C})$  for methyl H atoms. A rotating model was used for the methyl groups.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.37406 (10)	0.29201 (18)	0.92689 (19)	0.0762 (6)
H1A	0.3622	0.2494	0.9966	0.114*
H1B	0.3392	0.3247	0.8740	0.114*
H1C	0.4013	0.3482	0.9651	0.114*
C2	0.40429 (7)	0.21998 (14)	0.84101 (16)	0.0561 (4)
C3	0.41421 (6)	0.26245 (11)	0.71114 (14)	0.0431 (3)
C4	0.42533 (6)	0.19789 (12)	0.61119 (15)	0.0457 (3)
C5	0.45892 (6)	0.35303 (12)	0.49448 (16)	0.0479 (4)
C6	0.41194 (6)	0.38466 (11)	0.69024 (14)	0.0416 (3)
H6	0.4274	0.4189	0.7762	0.050*
C7	0.42452 (8)	0.07574 (13)	0.6116 (2)	0.0642 (5)
H7A	0.4647	0.0487	0.6187	0.096*
H7B	0.4005	0.0499	0.5304	0.096*
H7C	0.4078	0.0503	0.6859	0.096*
C8	0.43732 (9)	0.18379 (16)	0.37151 (19)	0.0668 (5)
H8A	0.4576	0.2249	0.3116	0.080*
H8B	0.4586	0.1154	0.3915	0.080*
C9	0.37589 (10)	0.16135 (14)	0.30636 (17)	0.0616 (5)
C10	0.32600 (12)	0.14343 (18)	0.2591 (2)	0.0814 (6)
H10	0.2863	0.1292	0.2215	0.098*
C11	0.34962 (6)	0.43142 (11)	0.64005 (14)	0.0416 (3)
C12	0.33358 (8)	0.52996 (13)	0.68949 (18)	0.0598 (4)
H12	0.3606	0.5657	0.7547	0.072*
C13	0.27831 (9)	0.57605 (15)	0.6439 (2)	0.0710 (5)
H13	0.2682	0.6419	0.6793	0.085*
C14	0.23830 (8)	0.52553 (16)	0.54682 (19)	0.0661 (5)
H14	0.2010	0.5569	0.5159	0.079*
C15	0.25341 (8)	0.42845 (17)	0.49538 (18)	0.0654 (5)
H15	0.2264	0.3942	0.4288	0.078*
C16	0.30871 (7)	0.38075 (14)	0.54179 (16)	0.0540 (4)
H16	0.3184	0.3144	0.5068	0.065*
N1	0.43908 (6)	0.24585 (10)	0.49518 (13)	0.0492 (3)
N2	0.45282 (5)	0.41268 (10)	0.60009 (13)	0.0475 (3)
H2	0.4741	0.4709	0.6161	0.057*
O1	0.42141 (8)	0.12989 (12)	0.88272 (15)	0.0905 (5)
O2	0.48212 (6)	0.38750 (10)	0.40209 (12)	0.0675 (4)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0941 (14)	0.0835 (14)	0.0571 (11)	−0.0056 (11)	0.0301 (10)	0.0089 (10)
C2	0.0586 (9)	0.0570 (9)	0.0511 (9)	−0.0103 (7)	0.0057 (7)	0.0122 (7)

C3	0.0382 (7)	0.0428 (7)	0.0473 (8)	-0.0046 (5)	0.0048 (6)	0.0070 (6)
C4	0.0380 (7)	0.0426 (7)	0.0560 (9)	-0.0023 (6)	0.0071 (6)	0.0068 (6)
C5	0.0386 (7)	0.0504 (8)	0.0552 (9)	-0.0059 (6)	0.0101 (6)	0.0078 (7)
C6	0.0413 (7)	0.0419 (7)	0.0404 (7)	-0.0077 (5)	0.0039 (6)	0.0016 (6)
C7	0.0699 (11)	0.0420 (8)	0.0797 (12)	0.0004 (8)	0.0107 (9)	0.0044 (8)
C8	0.0777 (12)	0.0605 (10)	0.0713 (11)	-0.0010 (9)	0.0380 (10)	-0.0101 (9)
C9	0.0905 (14)	0.0508 (9)	0.0465 (9)	-0.0035 (9)	0.0206 (9)	-0.0069 (7)
C10	0.1027 (17)	0.0762 (14)	0.0599 (12)	-0.0077 (12)	0.0005 (11)	-0.0086 (10)
C11	0.0432 (7)	0.0411 (7)	0.0405 (7)	-0.0043 (6)	0.0077 (6)	0.0031 (6)
C12	0.0630 (10)	0.0492 (9)	0.0643 (10)	-0.0009 (7)	0.0040 (8)	-0.0085 (8)
C13	0.0704 (12)	0.0539 (10)	0.0884 (14)	0.0140 (9)	0.0133 (10)	-0.0021 (10)
C14	0.0553 (10)	0.0698 (12)	0.0730 (12)	0.0148 (8)	0.0107 (9)	0.0146 (9)
C15	0.0486 (9)	0.0828 (13)	0.0600 (10)	0.0009 (8)	-0.0028 (8)	-0.0049 (9)
C16	0.0482 (8)	0.0573 (9)	0.0546 (9)	-0.0004 (7)	0.0039 (7)	-0.0107 (7)
N1	0.0504 (7)	0.0467 (7)	0.0537 (7)	-0.0039 (5)	0.0180 (6)	-0.0010 (6)
N2	0.0425 (6)	0.0443 (6)	0.0556 (8)	-0.0130 (5)	0.0087 (5)	0.0035 (6)
O1	0.1257 (13)	0.0719 (9)	0.0762 (9)	0.0121 (8)	0.0239 (9)	0.0339 (8)
O2	0.0714 (8)	0.0715 (8)	0.0659 (7)	-0.0185 (6)	0.0294 (6)	0.0075 (6)

*Geometric parameters (Å, °)*

C1—C2	1.495 (3)	C8—C9	1.457 (3)
C1—H1A	0.9600	C8—N1	1.470 (2)
C1—H1B	0.9600	C8—H8A	0.9700
C1—H1C	0.9600	C8—H8B	0.9700
C2—O1	1.222 (2)	C9—C10	1.167 (3)
C2—C3	1.480 (2)	C10—H10	0.9300
C3—C4	1.351 (2)	C11—C12	1.383 (2)
C3—C6	1.5131 (19)	C11—C16	1.385 (2)
C4—N1	1.4075 (19)	C12—C13	1.377 (2)
C4—C7	1.498 (2)	C12—H12	0.9300
C5—O2	1.2349 (18)	C13—C14	1.366 (3)
C5—N2	1.331 (2)	C13—H13	0.9300
C5—N1	1.3892 (19)	C14—C15	1.369 (3)
C6—N2	1.4600 (17)	C14—H14	0.9300
C6—C11	1.5248 (19)	C15—C16	1.387 (2)
C6—H6	0.9800	C15—H15	0.9300
C7—H7A	0.9600	C16—H16	0.9300
C7—H7B	0.9600	N2—H2	0.8600
C7—H7C	0.9600		
C2—C1—H1A	109.5	C9—C8—H8A	109.3
C2—C1—H1B	109.5	N1—C8—H8A	109.3
H1A—C1—H1B	109.5	C9—C8—H8B	109.3
C2—C1—H1C	109.5	N1—C8—H8B	109.3
H1A—C1—H1C	109.5	H8A—C8—H8B	108.0
H1B—C1—H1C	109.5	C10—C9—C8	177.27 (19)
O1—C2—C3	122.76 (17)	C9—C10—H10	180.0

O1—C2—C1	118.65 (16)	C12—C11—C16	118.11 (14)
C3—C2—C1	118.55 (15)	C12—C11—C6	119.59 (13)
C4—C3—C2	123.42 (14)	C16—C11—C6	122.25 (13)
C4—C3—C6	118.66 (13)	C13—C12—C11	121.18 (16)
C2—C3—C6	117.92 (13)	C13—C12—H12	119.4
C3—C4—N1	119.44 (13)	C11—C12—H12	119.4
C3—C4—C7	125.43 (14)	C14—C13—C12	120.28 (17)
N1—C4—C7	115.12 (14)	C14—C13—H13	119.9
O2—C5—N2	123.52 (14)	C12—C13—H13	119.9
O2—C5—N1	120.68 (15)	C13—C14—C15	119.60 (17)
N2—C5—N1	115.77 (13)	C13—C14—H14	120.2
N2—C6—C3	108.24 (11)	C15—C14—H14	120.2
N2—C6—C11	110.69 (11)	C14—C15—C16	120.55 (17)
C3—C6—C11	115.19 (11)	C14—C15—H15	119.7
N2—C6—H6	107.5	C16—C15—H15	119.7
C3—C6—H6	107.5	C11—C16—C15	120.29 (16)
C11—C6—H6	107.5	C11—C16—H16	119.9
C4—C7—H7A	109.5	C15—C16—H16	119.9
C4—C7—H7B	109.5	C5—N1—C4	121.35 (13)
H7A—C7—H7B	109.5	C5—N1—C8	116.37 (13)
C4—C7—H7C	109.5	C4—N1—C8	122.15 (13)
H7A—C7—H7C	109.5	C5—N2—C6	123.52 (12)
H7B—C7—H7C	109.5	C5—N2—H2	118.2
C9—C8—N1	111.51 (13)	C6—N2—H2	118.2

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C7—H7C $\cdots$ O1	0.96	2.21	2.862 (3)	125
N2—H2 $\cdots$ O2 <sup>i</sup>	0.86	2.02	2.8612 (17)	164

Symmetry code: (i)  $-x+1, -y+1, -z+1$ .