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

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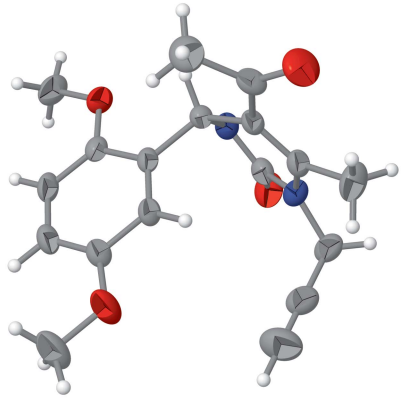
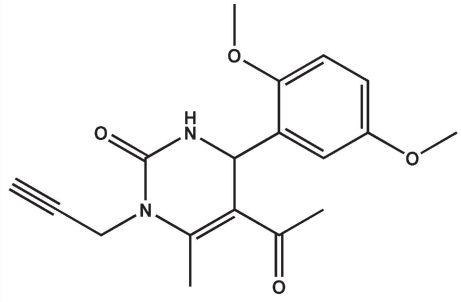
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{20}N_2O_4$, the 3,4-dihydropyrimidin-2(1*H*)-one ring has a screw-boat conformation. The mean plane through this heterocycle is almost perpendicular to the prop-2-ynyl chain and to the benzene ring, with which it makes a dihedral angle of 87.63 (6)°. The plane through the acetyl group makes a dihedral angle of 33.11 (8)° with the mean plane of the heterocycle. There is an intramolecular C—H···O hydrogen bond present forming an *S*(6) ring motif. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming layers parallel to the *bc* plane. There are also C—H···π interactions present within the layers.

3D view



Chemical scheme



Structure description

Dihydropyrimidinones (DHPMs) and their derivatives have received much attention because of their biological activities and widespread pharmacological activities, such as antiviral, antibacterial, antitumor and antihypertensive (Rovnyak *et al.*, 1995). Some have been used successfully as calcium channel blockers, α1a-antagonists and neuropeptide Y (NPY) antagonists (Atwal *et al.*, 1990). Several alkaloids, which contain the dihydropyrimidine core unit, have been isolated from marine sources. Most notable among these are the batzelladine alkaloids, which were found to be potent HIVgp-120-CD4 inhibitors (Snider *et al.*, 1996).

In connection with our studies, we chose to work on DHPMs, which have six possible sites around the DHPM ring where modification/functionalization can be achieved. Therefore, we decided to explore the feasibility of alkylated DHPMs. Thus, this investigation had allowed us to describe a new efficient method for the preparation of new compounds with regioselective N1-alkylation and N1/N3-bis-alkylation of DHPMs analogues (Mohamadpour *et al.*, 2016; Zare & Nasouri 2016).

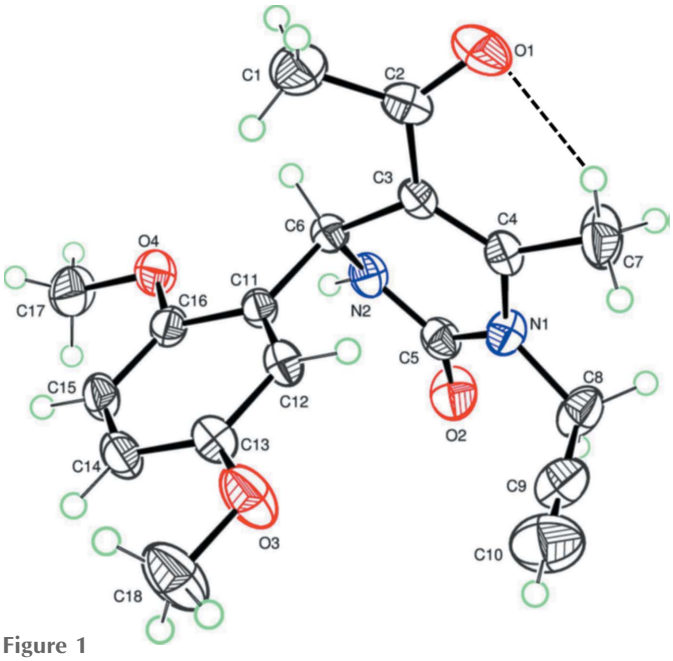


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular C—H···O hydrogen bond is shown as a dashed lines (see Table 1).

The molecule of the title compound (Fig. 1) is built up from a 3,4-dihydropyrimidin-2(1*H*)-one ring linked to an acetyl group, a prop-2-ynyl chain and a 2,5-dimethoxyphenyl group. The dihydropyrimidine ring (atoms N1/N2/C3–C6) adopts a screw-boat conformation, as indicated by the puckering parameters: $Q2$ = 0.4086 (13) Å, θ = 69.29 (18)° and φ = 196.6 (2)°. The dihedral angle between the mean plane of the heterocycle and that of the benzene ring is 87.63 (6)°. The prop-2-ynyl chain is nearly perpendicular to the mean plane of the dihydropyrimidine ring, with a C9—C8—N1—C4 torsion angle of −72.09 (19)°. There is an intramolecular C—H···O hydrogen bond present, forming an *S*(6) ring motif (Fig. 1 and Table 1).

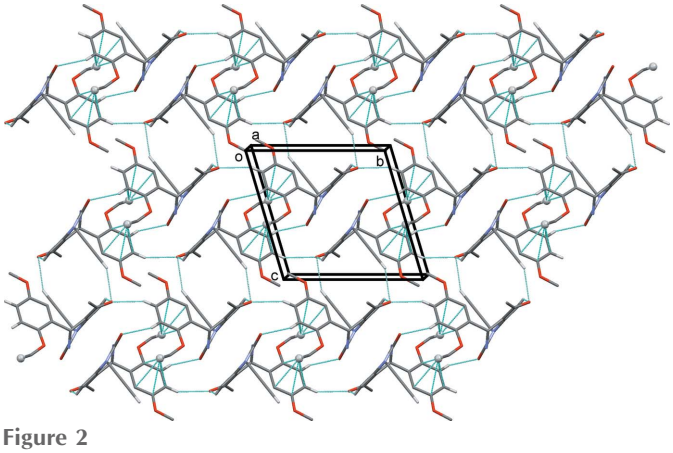


Figure 2
The crystal packing of the title compound, viewed along the *a* axis, showing molecules linked through C—H···O hydrogen bonds and C—H···π interactions (dashed lines; see Table 1). For clarity, only H atoms involved in these interactions have been included.

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

*Cg*1 is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O1	0.96	2.18	2.881 (2)	129
C10—H10···O1^{i}	0.93	2.57	3.406 (2)	150
C14—H14···O1^{ii}	0.93	2.60	3.393 (2)	144
C15—H15···O2^{iii}	0.93	2.55	3.437 (2)	161
C17—H17*A*···*Cg*1^{iii}	0.96	2.77	3.601 (2)	146

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_2O_4$
M_r	328.36
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	8.5948 (15), 10.1942 (16), 10.2572 (17)
α, β, γ (°)	74.930 (7), 75.306 (7), 89.866 (7)
V (Å^3)	837.5 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.27 × 0.24
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.587, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25426, 4005, 3333
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.658
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.147, 1.05
No. of reflections	4005
No. of parameters	221
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.24

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

In the crystal, molecules are linked by C—H···O hydrogen bonds, forming layers parallel to the *bc* plane. There are also C—H···π interactions present within the layers (Fig. 2 and Table 1).

Synthesis and crystallization

The title compound was prepared in good yield (70%) through condensation of 5-acetyl-4-(2,5-dimethoxyphenyl)-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one with propargyl bromide in the presence of potassium *tert*-butoxide in dry dimethylformamide at room temperature. The mixture was heated with stirring for 1 h. The crude product obtained was purified using a column packed with silica gel. The title compound was crystallized by slow evaporation from a solution in methanol (m.p. 428 K). ^{1}H NMR (DMSO-d_6): δ 2.08 (*s*, 3H, CH_3CO),

2.50 (*s*, 3H, CH_3), 3.28 (*s*, 1H, CH), 3.65 (*s*, 3H, OCH_3), 3.76 (*s*, 3H, OCH_3), 4.34–4.68 (*m*, 2H, –CH_2–), 5.49 (*s*, 1H, H-4), 6.64–6.65 (*s*, 1H), 6.65–6.95 (*m*, 2H, C—Ar), 7.80 (*s*, 1H, N3—H). The signal due to N1—H was not observable in the ^{1}H NMR spectrum. ^{13}C NMR (DMSO-d_6): δ 196.34 (CO), 153.19 (C-6), 152.25, 150.07, 146.45, 131.27, 113.29 (C-Ar), 112.30 (C-5), 80.51 (C-alkyl), 74.25 (CH-alkyl), 55.82 (OCH_3), 55.34 (OCH_3), 47.72 (C-4), 31.44 (–CH_3-), 29.63 (CH_3 at C-4′), 15.72 (CH_3 at C-6).

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**, x170816 [https://doi.org/10.1107/S2414314617008161]

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Crystal data

$C_{18}H_{20}N_2O_4$
M_r = 328.36
Triclinic, $P\overline{1}$
a = 8.5948 (15) Å
b = 10.1942 (16) Å
c = 10.2572 (17) Å
α = 74.930 (7)°
β = 75.306 (7)°
γ = 89.866 (7)°
V = 837.5 (2) Å^3
Z = 2
$F(000)$ = 348
D_x = 1.302 Mg m^{-3}
Melting point: 428 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4005 reflections
θ = 2.5–27.9°
μ = 0.09 mm^{-1}
T = 296 K
Prism, colourless
0.35 × 0.27 × 0.24 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.587, T_{max} = 0.746
25426 measured reflections
4005 independent reflections
3333 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.9°, θ_{min} = 2.5°
h = −11→11
k = −13→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.147
S = 1.05
4005 reflections
221 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0844P)^2 + 0.1806P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5494 (2)	0.41801 (18)	0.84088 (19)	0.0558 (4)
H1A	0.5399	0.3684	0.9362	0.084*
H1B	0.5578	0.5139	0.8323	0.084*
H1C	0.6439	0.3936	0.7813	0.084*
C2	0.40293 (17)	0.38370 (13)	0.79841 (14)	0.0377 (3)
C3	0.33613 (15)	0.49333 (11)	0.70720 (13)	0.0306 (3)
C4	0.18163 (15)	0.48869 (12)	0.69912 (13)	0.0340 (3)
C5	0.24167 (17)	0.68119 (13)	0.48927 (14)	0.0365 (3)
C6	0.44451 (14)	0.61836 (11)	0.62095 (12)	0.0300 (3)
H6	0.5553	0.5908	0.5986	0.036*
C7	0.0526 (2)	0.38038 (17)	0.78715 (19)	0.0554 (4)
H7A	0.0955	0.3151	0.8526	0.083*
H7B	0.0153	0.3355	0.7281	0.083*
H7C	−0.0356	0.4210	0.8371	0.083*
C8	−0.03898 (17)	0.61963 (18)	0.61831 (17)	0.0489 (4)
H8A	−0.0515	0.6812	0.5325	0.059*
H8B	−0.0998	0.5345	0.6335	0.059*
C9	−0.1038 (2)	0.67832 (18)	0.73473 (18)	0.0537 (4)
C10	−0.1570 (3)	0.7250 (2)	0.8278 (2)	0.0772 (6)
H10	−0.1994	0.7623	0.9020	0.093*
C11	0.44181 (14)	0.73281 (11)	0.69222 (13)	0.0291 (3)
C12	0.32378 (15)	0.73776 (12)	0.80983 (13)	0.0335 (3)
H12	0.2438	0.6672	0.8507	0.040*
C13	0.32220 (17)	0.84719 (13)	0.86881 (14)	0.0363 (3)
C14	0.44185 (18)	0.95137 (13)	0.80889 (15)	0.0398 (3)
H14	0.4420	1.0242	0.8478	0.048*
C15	0.56169 (17)	0.94741 (13)	0.69075 (15)	0.0393 (3)
H15	0.6424	1.0175	0.6512	0.047*
C16	0.56234 (14)	0.83999 (12)	0.63111 (13)	0.0324 (3)
C17	0.79489 (19)	0.93614 (16)	0.44539 (19)	0.0546 (4)
H17A	0.7447	1.0193	0.4175	0.082*
H17B	0.8642	0.9166	0.3642	0.082*
H17C	0.8573	0.9456	0.5083	0.082*
C18	0.1949 (3)	0.94388 (18)	1.0534 (2)	0.0659 (5)
H18A	0.2918	0.9453	1.0834	0.099*
H18B	0.1031	0.9261	1.1332	0.099*
H18C	0.1879	1.0304	0.9905	0.099*
N1	0.13235 (13)	0.59452 (12)	0.60294 (12)	0.0377 (3)
N2	0.39836 (13)	0.66749 (11)	0.48902 (11)	0.0351 (3)

H2	0.4624	0.7272	0.4224	0.042*
O1	0.34499 (16)	0.26674 (10)	0.83972 (14)	0.0602 (3)
O2	0.19764 (15)	0.75801 (11)	0.39413 (12)	0.0547 (3)
O3	0.19759 (15)	0.84067 (11)	0.98417 (12)	0.0558 (3)
O4	0.67395 (11)	0.82756 (10)	0.51386 (11)	0.0428 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0623 (10)	0.0530 (9)	0.0600 (10)	0.0125 (7)	−0.0329 (8)	−0.0122 (7)
C2	0.0458 (7)	0.0295 (6)	0.0356 (6)	0.0060 (5)	−0.0065 (5)	−0.0090 (5)
C3	0.0346 (6)	0.0238 (5)	0.0328 (6)	−0.0012 (4)	−0.0066 (5)	−0.0085 (4)
C4	0.0359 (6)	0.0314 (6)	0.0345 (6)	−0.0041 (5)	−0.0072 (5)	−0.0106 (5)
C5	0.0444 (7)	0.0337 (6)	0.0354 (6)	0.0004 (5)	−0.0147 (5)	−0.0123 (5)
C6	0.0290 (6)	0.0268 (5)	0.0333 (6)	0.0007 (4)	−0.0068 (5)	−0.0080 (5)
C7	0.0465 (8)	0.0522 (9)	0.0584 (10)	−0.0194 (7)	−0.0119 (7)	−0.0009 (7)
C8	0.0353 (7)	0.0679 (10)	0.0505 (8)	0.0064 (7)	−0.0175 (6)	−0.0219 (7)
C9	0.0421 (8)	0.0653 (10)	0.0563 (9)	0.0110 (7)	−0.0154 (7)	−0.0186 (8)
C10	0.0824 (15)	0.0867 (15)	0.0677 (12)	0.0240 (12)	−0.0142 (11)	−0.0352 (11)
C11	0.0297 (6)	0.0244 (5)	0.0346 (6)	0.0000 (4)	−0.0133 (5)	−0.0056 (4)
C12	0.0358 (6)	0.0269 (5)	0.0365 (6)	−0.0050 (5)	−0.0085 (5)	−0.0071 (5)
C13	0.0425 (7)	0.0311 (6)	0.0358 (6)	−0.0003 (5)	−0.0099 (5)	−0.0100 (5)
C14	0.0471 (7)	0.0291 (6)	0.0478 (8)	−0.0022 (5)	−0.0172 (6)	−0.0134 (5)
C15	0.0373 (7)	0.0284 (6)	0.0514 (8)	−0.0075 (5)	−0.0150 (6)	−0.0060 (5)
C16	0.0281 (6)	0.0296 (6)	0.0387 (6)	−0.0005 (4)	−0.0118 (5)	−0.0047 (5)
C17	0.0374 (8)	0.0484 (8)	0.0628 (10)	−0.0105 (6)	−0.0009 (7)	−0.0006 (7)
C18	0.0874 (14)	0.0520 (9)	0.0549 (10)	−0.0101 (9)	0.0030 (9)	−0.0295 (8)
N1	0.0318 (5)	0.0425 (6)	0.0395 (6)	0.0005 (4)	−0.0116 (5)	−0.0098 (5)
N2	0.0371 (6)	0.0350 (5)	0.0298 (5)	−0.0051 (4)	−0.0048 (4)	−0.0066 (4)
O1	0.0716 (8)	0.0285 (5)	0.0726 (8)	0.0021 (5)	−0.0178 (6)	−0.0008 (5)
O2	0.0619 (7)	0.0534 (6)	0.0487 (6)	−0.0029 (5)	−0.0290 (5)	0.0006 (5)
O3	0.0667 (7)	0.0448 (6)	0.0493 (6)	−0.0138 (5)	0.0084 (5)	−0.0241 (5)
O4	0.0338 (5)	0.0388 (5)	0.0482 (6)	−0.0059 (4)	−0.0014 (4)	−0.0078 (4)

Geometric parameters (Å, º)

C1—C2	1.502 (2)	C9—C10	1.167 (3)
C1—H1A	0.9600	C10—H10	0.9300
C1—H1B	0.9600	C11—C12	1.3775 (18)
C1—H1C	0.9600	C11—C16	1.4070 (16)
C2—O1	1.2174 (17)	C12—C13	1.3991 (17)
C2—C3	1.4764 (17)	C12—H12	0.9300
C3—C4	1.3529 (18)	C13—O3	1.3668 (17)
C3—C6	1.5087 (16)	C13—C14	1.3814 (19)
C4—N1	1.4046 (17)	C14—C15	1.387 (2)
C4—C7	1.4978 (18)	C14—H14	0.9300
C5—O2	1.2237 (16)	C15—C16	1.3856 (18)
C5—N2	1.3530 (18)	C15—H15	0.9300

C5—N1	1.3912 (18)	C16—O4	1.3698 (16)
C6—N2	1.4691 (16)	C17—O4	1.4246 (17)
C6—C11	1.5267 (16)	C17—H17A	0.9600
C6—H6	0.9800	C17—H17B	0.9600
C7—H7A	0.9600	C17—H17C	0.9600
C7—H7B	0.9600	C18—O3	1.4110 (18)
C7—H7C	0.9600	C18—H18A	0.9600
C8—C9	1.458 (2)	C18—H18B	0.9600
C8—N1	1.4697 (18)	C18—H18C	0.9600
C8—H8A	0.9700	N2—H2	0.8572
C8—H8B	0.9700		

C2—C1—H1A	109.5	C12—C11—C16	119.07 (11)
C2—C1—H1B	109.5	C12—C11—C6	122.88 (10)
H1A—C1—H1B	109.5	C16—C11—C6	118.01 (11)
C2—C1—H1C	109.5	C11—C12—C13	121.09 (11)
H1A—C1—H1C	109.5	C11—C12—H12	119.5
H1B—C1—H1C	109.5	C13—C12—H12	119.5
O1—C2—C3	122.78 (13)	O3—C13—C14	125.23 (12)
O1—C2—C1	118.74 (13)	O3—C13—C12	115.32 (12)
C3—C2—C1	118.48 (12)	C14—C13—C12	119.45 (12)
C4—C3—C2	123.36 (11)	C13—C14—C15	120.03 (12)
C4—C3—C6	118.25 (11)	C13—C14—H14	120.0
C2—C3—C6	118.38 (11)	C15—C14—H14	120.0
C3—C4—N1	118.96 (11)	C16—C15—C14	120.61 (12)
C3—C4—C7	125.79 (13)	C16—C15—H15	119.7
N1—C4—C7	115.24 (12)	C14—C15—H15	119.7
O2—C5—N2	123.43 (13)	O4—C16—C15	125.03 (11)
O2—C5—N1	121.63 (13)	O4—C16—C11	115.24 (11)
N2—C5—N1	114.83 (11)	C15—C16—C11	119.73 (12)
N2—C6—C3	107.64 (10)	O4—C17—H17A	109.5
N2—C6—C11	110.29 (9)	O4—C17—H17B	109.5
C3—C6—C11	114.99 (10)	H17A—C17—H17B	109.5
N2—C6—H6	107.9	O4—C17—H17C	109.5
C3—C6—H6	107.9	H17A—C17—H17C	109.5
C11—C6—H6	107.9	H17B—C17—H17C	109.5
C4—C7—H7A	109.5	O3—C18—H18A	109.5
C4—C7—H7B	109.5	O3—C18—H18B	109.5
H7A—C7—H7B	109.5	H18A—C18—H18B	109.5
C4—C7—H7C	109.5	O3—C18—H18C	109.5
H7A—C7—H7C	109.5	H18A—C18—H18C	109.5
H7B—C7—H7C	109.5	H18B—C18—H18C	109.5
C9—C8—N1	111.79 (12)	C5—N1—C4	122.27 (11)
C9—C8—H8A	109.3	C5—N1—C8	116.49 (12)
N1—C8—H8A	109.3	C4—N1—C8	121.24 (12)
C9—C8—H8B	109.3	C5—N2—C6	120.61 (11)
N1—C8—H8B	109.3	C5—N2—H2	112.9
H8A—C8—H8B	107.9	C6—N2—H2	117.8

C10—C9—C8	179.4 (2)	C13—O3—C18	117.94 (13)
C9—C10—H10	180.0	C16—O4—C17	117.23 (11)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of ring C11-C16.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O1	0.96	2.18	2.881 (2)	129
C10—H10···O1^{i}	0.93	2.57	3.406 (2)	150
C14—H14···O1^{ii}	0.93	2.60	3.393 (2)	144
C15—H15···O2^{iii}	0.93	2.55	3.437 (2)	161
C17—H17*A*···*Cg*1^{iii}	0.96	2.77	3.601 (2)	146

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