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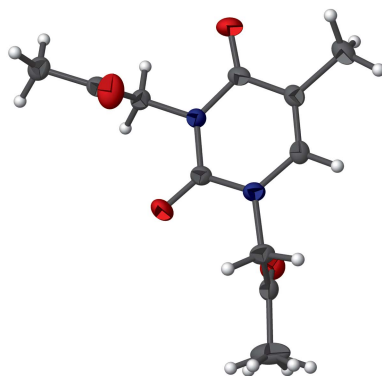
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

# 1,3-Bis(2-oxopropyl)thymine

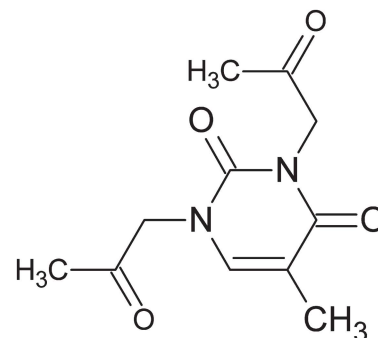
Bogdan Doboszewski,<sup>a</sup> Alexander Y. Nazarenko<sup>b\*</sup> and Fábio da Paixão Soares<sup>a</sup><sup>a</sup>Departamento de Química, Universidade Federal Rural de Pernambuco, 52171-900 Recife, PE, Brazil, and <sup>b</sup>Chemistry Department, State University of New York, College at Buffalo, 1300 Elmwood Ave, Buffalo, NY 14222-1095, USA.\*Correspondence e-mail: [nazareay@buffalostate.edu](mailto:nazareay@buffalostate.edu)

In the title compound [systematic name: 5-methyl-1,3-bis(2-oxopropyl)pyrimidine-2,4(1*H*,3*H*)-dione], C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>, the two 2-oxopropyl groups are nearly perpendicular to the planar thymine unit. One methyl group of oxopropyl substituent is disordered. In the crystal, C—H···O interactions help to connect the molecules into (001) layers.

## 3D view



## Chemical scheme



## Structure description

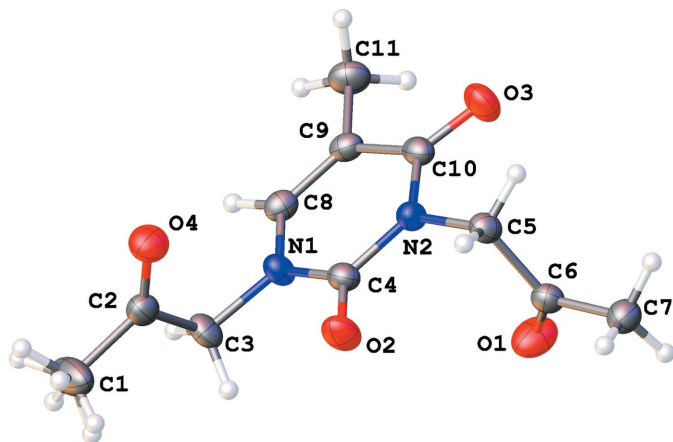
Nucleoside analogs play an important role in combating viral diseases and neoplasms; this is demonstrated by the pharmacological success of drugs such as Zidovudine, Stavudine, Lamivudine, and around 20 others belonging to this group of compounds (Adamska *et al.*, 2016; Krim *et al.*, 2012; Negrón-Silva *et al.*, 2013; Thakur *et al.*, 2014). We performed the transformation of *N*<sup>1</sup>,*N*<sup>3</sup>-bispropargyl thymine and uracyl, which furnished *N*<sup>1</sup>,*N*<sup>3</sup>-bis-(2-oxopro-1-yl) derivatives; these compounds offer ample possibilities of further functionalization *via* C or O alkylation of their enolates, or *via* reductive amination, among others.

In the title compound (Fig. 1), the thymine unit is nearly planar, with the largest deviation from the mean plane being less than 0.03 Å. The two essentially planar 2-oxopropyl substituents are almost perpendicular to the thymine unit; the dihedral angles between the mean plane of the six-membered ring and those of the 2-oxopropyl fragments with atoms C1 and C7 are 77.96 (1) and 82.92 (1)°, respectively. Rotational disorder was observed for the C1 methyl group of the 2-oxopropyl substituent.

There are no usual hydrogen bonds in this structure. Attractive C—H···O interactions (Table 1), involving all oxygen atoms of the molecule, help to organize the molecules in a layer parallel to the (001) plane. These layers are packed in the three-dimensional crystal by van der Waals forces, mainly between hydrogen atoms (Fig. 2).



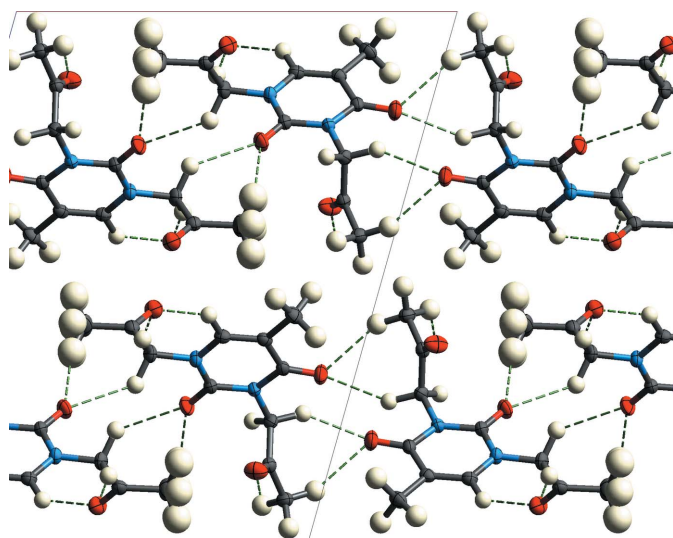
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**Figure 1**  
Numbering scheme for the title compound, shown with 50% probability displacement ellipsoids.

### Synthesis and crystallization

As *N1,N3*-bispropargyl thymine can be prepared in yields exceeding 80%, we used it as a starting material to obtain the title compound (**1**) *via* addition of water catalyzed by silica-supported  $\text{HgSO}_4/\text{H}_2\text{SO}_4$  (Mello *et al.*, 2010). This furnished the necessary **1** ( $R_f$  0.30, EtOAc neat, more polar than *N1,N3*-bis-propargylthymine,  $R_f$  0.70, hexane-EtOAc) by simple filtration of the solids and crystallization from ethyl acetate. The product formed well-resolved crystals suitable for X-ray analysis. Compound **1**: m.p. 408–412 K (EtOAc).  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}-d_6$ ): 7.47 (broadened *s*, 1H, H6), 4.66 and 4.64 (two *s*, total of 4H,  $\text{NCH}_2$ ), 2.16 and 2.14 (two *s*, total of 6H,  $\text{COCH}_3$ ), 1.80 (broadened *s*, 3H,  $\text{C}_5\text{CH}_3$ ).  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}-d_6$ ): 201.8 and 201.3 (two  $\text{COCH}_3$ ), 162.0 and 150.6 (C2, 4), 140.8 (C6), 107.3 (C5), 56.9 and 49.7 (two  $\text{CH}_2$ ), 27.1 and 26.8 (two  $\text{COCH}_3$ ), 12.4 ( $\text{C}_5\text{CH}_3$ ).



**Figure 2**  
Packing of the title compound, viewed along [010].

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3A}\cdots\text{O2}^i$	0.97 (1)	2.56 (1)	3.304 (2)	134 (1)
$\text{C3}-\text{H3B}\cdots\text{O4}^{ii}$	0.97 (1)	2.45 (1)	3.3820 (19)	160 (1)
$\text{C5}-\text{H5B}\cdots\text{O3}^{iii}$	0.96 (1)	2.50 (1)	3.353 (2)	148 (1)
$\text{C7}-\text{H7A}\cdots\text{O1}^{iv}$	0.96 (1)	2.54 (1)	3.2576 (19)	131 (1)
$\text{C7}-\text{H7B}\cdots\text{O3}^{iii}$	0.96 (1)	2.50 (1)	3.370 (2)	150 (1)
$\text{C8}-\text{H8}\cdots\text{O4}^{ii}$	0.96 (1)	2.50 (1)	3.3213 (19)	144 (1)

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

**Table 2**  
Experimental details.

Crystal data	$\text{C}_{11}\text{H}_{14}\text{N}_2\text{O}_4$
Chemical formula	238.24
$M_r$	Monoclinic, $P2_1/c$
Crystal system, space group	173
Temperature (K)	13.9490 (9), 4.9891 (3), 17.3647 (11)
$a, b, c$ ( $\text{\AA}$ )	105.693 (4)
$\beta$ ( $^\circ$ )	1163.41 (13)
$V$ ( $\text{\AA}^3$ )	4
$Z$	Mo $K\alpha$
Radiation type	0.11
$\mu$ ( $\text{mm}^{-1}$ )	0.2 $\times$ 0.15 $\times$ 0.08
Crystal size (mm)	
Data collection	
Diffractometer	Bruker PHOTON-100 CMOS
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\min}, T_{\max}$	0.769, 0.862
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	18736, 2458, 1889
$R_{\text{int}}$	0.051
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.632
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.103, 1.03
No. of reflections	2458
No. of parameters	163
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.21, -0.19

Computer programs: *APEX2* (Bruker, 2013) *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Methyl group C1 is disordered.

### Acknowledgements

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## full crystallographic data

*IUCrData* (2020). 5, x200257 [https://doi.org/10.1107/S2414314620002576]

## 1,3-Bis(2-oxopropyl)thymine

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5-Methyl-1,3-bis(2-oxopropyl)pyrimidine-2,4(1*H*,3*H*)-dione*Crystal data*

$C_{11}H_{14}N_2O_4$

$M_r = 238.24$

Monoclinic,  $P2_1/c$

$a = 13.9490$  (9) Å

$b = 4.9891$  (3) Å

$c = 17.3647$  (11) Å

$\beta = 105.693$  (4)°

$V = 1163.41$  (13) Å<sup>3</sup>

$Z = 4$

$F(000) = 504$

$D_x = 1.360$  Mg m<sup>-3</sup>

Melting point: 412 K

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

Cell parameters from 2683 reflections

$\theta = 3.0$ – $25.8$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 173$  K

Plate, colourless

$0.2 \times 0.15 \times 0.08$  mm

*Data collection*

Bruker PHOTON-100 CMOS  
diffractometer

Radiation source: sealedtube

Detector resolution: 10.4 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.769$ ,  $T_{\max} = 0.862$

18736 measured reflections

2458 independent reflections

1889 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 26.7$ °,  $\theta_{\min} = 3.0$ °

$h = -17 \rightarrow 17$

$k = -6 \rightarrow 6$

$l = -21 \rightarrow 21$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.103$

$S = 1.03$

2458 reflections

163 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.5355P]$

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

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

$\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.18$  e Å<sup>-3</sup>

*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.** Methylene hydrogen atoms are refined with riding coordinates and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{iso}}(\text{C})$ ; methyl hydrogen atoms are refined as rotating idealized methyl groups and with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{iso}}(\text{C})$ .

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.83624 (10)	0.9143 (2)	0.36977 (7)	0.0433 (3)	
O2	0.63791 (8)	1.2059 (2)	0.24695 (7)	0.0361 (3)	
O3	0.92187 (8)	0.9349 (2)	0.18756 (7)	0.0378 (3)	
O4	0.50121 (8)	1.2301 (2)	0.06408 (7)	0.0364 (3)	
N1	0.62809 (9)	0.8661 (3)	0.15811 (7)	0.0258 (3)	
N2	0.78007 (9)	1.0765 (3)	0.21574 (7)	0.0244 (3)	
C1	0.35466 (13)	1.0758 (5)	0.09457 (13)	0.0579 (6)	
H1A	0.333498	1.262010	0.097365	0.087*	0.43 (3)
H1B	0.343268	0.974481	0.139636	0.087*	0.43 (3)
H1C	0.316192	0.995262	0.044202	0.087*	0.43 (3)
H1D	0.328474	0.892492	0.090103	0.087*	0.57 (3)
H1E	0.318704	1.180021	0.047833	0.087*	0.57 (3)
H1F	0.345780	1.159240	0.143267	0.087*	0.57 (3)
C2	0.46300 (11)	1.0691 (3)	0.09839 (9)	0.0285 (4)	
C3	0.52141 (11)	0.8459 (3)	0.14837 (10)	0.0291 (4)	
H3A	0.50906 (19)	0.8483 (3)	0.2009 (7)	0.035*	
H3B	0.4978 (3)	0.675 (2)	0.1234 (3)	0.035*	
C4	0.67906 (11)	1.0595 (3)	0.20955 (9)	0.0252 (3)	
C5	0.83796 (11)	1.2601 (3)	0.27622 (8)	0.0261 (3)	
H5A	0.8008 (5)	1.422 (2)	0.27574 (8)	0.031*	
H5B	0.8985 (8)	1.3054 (7)	0.26324 (18)	0.031*	
C6	0.86268 (11)	1.1388 (3)	0.35899 (9)	0.0266 (3)	
C7	0.91998 (12)	1.3150 (3)	0.42473 (9)	0.0316 (4)	
H7A	0.8774 (5)	1.456 (2)	0.4341 (5)	0.047*	
H7B	0.9756 (8)	1.392 (2)	0.4098 (3)	0.047*	
H7C	0.9440 (8)	1.2108 (12)	0.4727 (6)	0.047*	
C8	0.67438 (11)	0.7030 (3)	0.11540 (9)	0.0259 (3)	
H8	0.6350 (7)	0.574 (2)	0.0796 (7)	0.031*	
C9	0.77188 (11)	0.7166 (3)	0.12144 (8)	0.0250 (3)	
C10	0.83202 (11)	0.9100 (3)	0.17581 (9)	0.0254 (3)	
C11	0.82282 (13)	0.5375 (4)	0.07549 (10)	0.0347 (4)	
H11A	0.7752 (6)	0.398 (2)	0.0469 (7)	0.052*	
H11B	0.8811 (8)	0.449 (2)	0.1132 (4)	0.052*	
H11C	0.8461 (8)	0.6461 (12)	0.0358 (6)	0.052*	

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0613 (9)	0.0324 (7)	0.0357 (7)	−0.0108 (6)	0.0122 (6)	0.0031 (5)
O2	0.0298 (6)	0.0419 (7)	0.0409 (7)	−0.0006 (5)	0.0169 (5)	−0.0137 (6)
O3	0.0215 (6)	0.0471 (8)	0.0452 (7)	0.0015 (5)	0.0095 (5)	−0.0046 (6)
O4	0.0377 (7)	0.0335 (7)	0.0383 (7)	−0.0051 (5)	0.0108 (5)	0.0024 (5)

N1	0.0200 (6)	0.0270 (7)	0.0309 (7)	-0.0016 (5)	0.0079 (5)	-0.0025 (6)
N2	0.0212 (6)	0.0294 (7)	0.0234 (6)	-0.0016 (5)	0.0073 (5)	-0.0028 (5)
C1	0.0299 (10)	0.0888 (17)	0.0564 (12)	0.0140 (10)	0.0142 (9)	0.0332 (12)
C2	0.0279 (8)	0.0338 (9)	0.0241 (7)	-0.0036 (7)	0.0075 (6)	-0.0053 (7)
C3	0.0213 (8)	0.0303 (9)	0.0366 (9)	-0.0047 (6)	0.0093 (6)	-0.0001 (7)
C4	0.0221 (7)	0.0288 (8)	0.0260 (7)	-0.0009 (6)	0.0086 (6)	0.0001 (6)
C5	0.0242 (8)	0.0285 (8)	0.0255 (8)	-0.0042 (6)	0.0064 (6)	-0.0023 (6)
C6	0.0237 (8)	0.0296 (8)	0.0278 (8)	0.0008 (6)	0.0091 (6)	0.0004 (7)
C7	0.0313 (9)	0.0361 (9)	0.0262 (8)	-0.0022 (7)	0.0058 (6)	0.0011 (7)
C8	0.0302 (8)	0.0248 (8)	0.0227 (7)	-0.0013 (6)	0.0074 (6)	-0.0010 (6)
C9	0.0295 (8)	0.0249 (8)	0.0217 (7)	0.0038 (6)	0.0087 (6)	0.0028 (6)
C10	0.0222 (8)	0.0304 (8)	0.0246 (7)	0.0038 (6)	0.0081 (6)	0.0050 (6)
C11	0.0383 (9)	0.0361 (10)	0.0340 (9)	0.0054 (8)	0.0168 (7)	-0.0022 (8)

*Geometric parameters (Å, °)*

O1—C6	1.2093 (19)	C2—C3	1.508 (2)
O2—C4	1.2191 (18)	C3—H3A	0.972 (12)
O3—C10	1.2205 (18)	C3—H3B	0.972 (12)
O4—C2	1.2066 (19)	C5—H5A	0.958 (12)
N1—C3	1.4551 (19)	C5—H5B	0.958 (12)
N1—C4	1.3749 (19)	C5—C6	1.511 (2)
N1—C8	1.3742 (19)	C6—C7	1.491 (2)
N2—C4	1.3864 (18)	C7—H7A	0.962 (10)
N2—C5	1.4612 (19)	C7—H7B	0.962 (10)
N2—C10	1.4027 (19)	C7—H7C	0.962 (10)
C1—H1A	0.9800	C8—H8	0.959 (17)
C1—H1B	0.9800	C8—C9	1.337 (2)
C1—H1C	0.9800	C9—C10	1.449 (2)
C1—H1D	0.9800	C9—C11	1.499 (2)
C1—H1E	0.9800	C11—H11A	0.997 (11)
C1—H1F	0.9800	C11—H11B	0.997 (11)
C1—C2	1.495 (2)	C11—H11C	0.997 (11)
C4—N1—C3	117.21 (12)	H3A—C3—H3B	107.8
C8—N1—C3	120.74 (13)	O2—C4—N1	122.08 (13)
C8—N1—C4	122.02 (12)	O2—C4—N2	122.48 (14)
C4—N2—C5	116.53 (12)	N1—C4—N2	115.44 (13)
C4—N2—C10	125.13 (13)	N2—C5—H5A	109.2
C10—N2—C5	117.87 (12)	N2—C5—H5B	109.2
H1A—C1—H1B	109.5	N2—C5—C6	111.84 (13)
H1A—C1—H1C	109.5	H5A—C5—H5B	107.9
H1A—C1—H1D	141.1	C6—C5—H5A	109.2
H1A—C1—H1E	56.3	C6—C5—H5B	109.2
H1A—C1—H1F	56.3	O1—C6—C5	121.18 (14)
H1B—C1—H1C	109.5	O1—C6—C7	123.40 (14)
H1B—C1—H1D	56.3	C7—C6—C5	115.42 (13)
H1B—C1—H1E	141.1	C6—C7—H7A	109.5

H1B—C1—H1F	56.3	C6—C7—H7B	109.5
H1C—C1—H1D	56.3	C6—C7—H7C	109.5
H1C—C1—H1E	56.3	H7A—C7—H7B	109.5
H1C—C1—H1F	141.1	H7A—C7—H7C	109.5
H1D—C1—H1E	109.5	H7B—C7—H7C	109.5
H1D—C1—H1F	109.5	N1—C8—H8	118.5
H1E—C1—H1F	109.5	C9—C8—N1	122.96 (14)
C2—C1—H1A	109.5	C9—C8—H8	118.5
C2—C1—H1B	109.5	C8—C9—C10	118.83 (14)
C2—C1—H1C	109.5	C8—C9—C11	123.13 (14)
C2—C1—H1D	109.5	C10—C9—C11	118.03 (13)
C2—C1—H1E	109.5	O3—C10—N2	120.12 (14)
C2—C1—H1F	109.5	O3—C10—C9	124.33 (14)
O4—C2—C1	122.64 (16)	N2—C10—C9	115.55 (12)
O4—C2—C3	122.26 (14)	C9—C11—H11A	109.5
C1—C2—C3	115.10 (14)	C9—C11—H11B	109.5
N1—C3—C2	113.07 (13)	C9—C11—H11C	109.5
N1—C3—H3A	109.0	H11A—C11—H11B	109.5
N1—C3—H3B	109.0	H11A—C11—H11C	109.5
C2—C3—H3A	109.0	H11B—C11—H11C	109.5
C2—C3—H3B	109.0		
O4—C2—C3—N1	6.9 (2)	C5—N2—C4—O2	6.5 (2)
N1—C8—C9—C10	0.5 (2)	C5—N2—C4—N1	-173.64 (13)
N1—C8—C9—C11	179.45 (14)	C5—N2—C10—O3	-5.4 (2)
N2—C5—C6—O1	0.6 (2)	C5—N2—C10—C9	175.01 (12)
N2—C5—C6—C7	-178.80 (12)	C8—N1—C3—C2	-103.59 (16)
C1—C2—C3—N1	-173.11 (16)	C8—N1—C4—O2	179.34 (15)
C3—N1—C4—O2	1.3 (2)	C8—N1—C4—N2	-0.5 (2)
C3—N1—C4—N2	-178.54 (13)	C8—C9—C10—O3	178.02 (15)
C3—N1—C8—C9	179.04 (14)	C8—C9—C10—N2	-2.5 (2)
C4—N1—C3—C2	74.43 (17)	C10—N2—C4—O2	178.41 (14)
C4—N1—C8—C9	1.1 (2)	C10—N2—C4—N1	-1.7 (2)
C4—N2—C5—C6	79.50 (16)	C10—N2—C5—C6	-93.04 (15)
C4—N2—C10—O3	-177.28 (14)	C11—C9—C10—O3	-1.0 (2)
C4—N2—C10—C9	3.2 (2)	C11—C9—C10—N2	178.53 (13)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3A $\cdots$ O2 <sup>i</sup>	0.97 (1)	2.56 (1)	3.304 (2)	134 (1)
C3—H3B $\cdots$ O4 <sup>ii</sup>	0.97 (1)	2.45 (1)	3.3820 (19)	160 (1)
C5—H5B $\cdots$ O3 <sup>iii</sup>	0.96 (1)	2.50 (1)	3.353 (2)	148 (1)
C7—H7A $\cdots$ O1 <sup>iv</sup>	0.96 (1)	2.54 (1)	3.2576 (19)	131 (1)
C7—H7B $\cdots$ O3 <sup>iii</sup>	0.96 (1)	2.50 (1)	3.370 (2)	150 (1)
C8—H8 $\cdots$ O4 <sup>ii</sup>	0.96 (1)	2.50 (1)	3.3213 (19)	144 (1)

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