Two polyacetylated 6-amino-5-[*N*-($^\beta$-D-glucopyranosyl)amino]-3-methylpyrimidine-2,4(1*H*,3*H*)-diones

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Abstract

The relative orientations of the pyrimidine base and pyranoside sugar moieties in 6-amino-5-*N*-acetyl-N-(β-*D*-3,4,6-tri-*O*-acetylglucopyranosyl)- amino-3-methylpyrimidine-2,4(1*H*)-dione hydrate, $C_{19}H_{26}N_4O_{11} \cdot H_2O$, (I), and in 6-acetamido-5-*N*-acetyl-N-(β-*D*-2,3,4,6-tetra-*O*-acetylgluco- pyranosyl)amino-3-methylpyrimidine-2,4(1*H*)-dione, $C_{23}H_{30}N_3O_{13}$, (II), are primarily determined by intramolecular N—H···O and O—H···O hydrogen bonds in (I), and by an N—H···O hydrogen bond in (II).

Comment

Two different polyacetylated derivatives of 6-amino-5-N-(β-*D*-glucopyranosyl)amino-3-methylpyrimidine-2,4(1*H*,3H)-di-one were prepared through different reaction conditions leading to different degrees of acetylation. A paper describing the chemistry is in preparation.

In $C_{19}H_{26}N_4O_{11} \cdot H_2O$, (I), the amino group of the pyrimidine base forms an N—H···O bond to the sugar ring oxygen [N6···O6' 3.015 (5) Å] and the free sugar O—H group forms an O—H···O hydrogen bond with an adjacent pyrimidine keto oxygen [O2'···O4 2.678 (5) Å]. The remaining two N—H groups in (I) and the O—H groups of the water molecule serve as donors in a three-dimensional hydrogen-bond network.

In $C_{23}H_{30}N_3O_{13}$, (II), there is only an N—H···O hydrogen bond between the pyrimidine base and the sugar ring [N6···O6' 2.910 (4) Å]; a further N—H···O hydrogen bond controls the orientation of the 6-acetamido group [N1···O62 2.680 (4) Å]. Interactions between molecules correspond with normal van der Waals interactions.

Experimental

Preparation of (I): 4 ml of pyridine and 4 ml of acetic anhydride were added to a suspension of 0.41 g of 6-amino-5-N-(β-*D*-glucopyranosyl)amino-3- methylpyrimidine-2,4(1*H*,3*H*)-dione and the resulting mixture was stirred at room temperature until it dissolved then left to stand for 1 d. Removal of the solvent resulted in a solid which was dissolved in 20 ml of chloroform and then washed subsequently with 20 ml of aqueous dilute HCl solution, 20 ml of a aqueous dilute $NaHCO_3$ solution and finally with 20 ml or water. The final organic phase was dried over anhydrous sodium sulfate, the solvent removed giving a solid, which was re-crystallized from water (49% yield, m.p. 525 K).

Preparation of (II): 1 g of 6-amino-5-N-(β-*D*-glucopyranosyl)amino-3- methylpyrimidine-2,4(1*H*,3*H*)-dione was heated at 353 K in a mixture of 25 ml of acetic anhydride and a drop of perchloric acid until dissolved. The reaction mixture was then cooled to room temperature and left to stand for 1 d. The mixture was processed as described for (I) above to give solid (II), which was crystallized from ethanol (45% yield, m.p. 528 K).

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Refinement

Compounds (I) and (II) crystallized in the orthorhombic system; space group $P2_12_12_1$ from the systematic absences. Friedel pairs were merged before refinement since the molecules contained only C, H, N and O atoms. The H atoms attached to the water solvent molecule in (I) were located on difference map and then restrained to a bond length of 0.90 (2)Å by use of a *DFIX* command. All other H atoms were treated as riding atoms (C—H 0.93 to 0.98, N—H 0.86, O—H 0.82 Å). Difference maps showed that some of the methyl H atoms were disordered and these were allowed for as six evenly spaced 0.5 occupancy H atoms. Examination of the structures with *PLATON* (Spek, 1999) showed that there were no solvent accessible voids in the crystal lattice.

Computing details

For both compounds, data collection: *CAD-4-PC* Software (Enraf-Nonius, 1992); cell refinement: *SET4* and *CELDIM* (Enraf-Nonius, 1992); data reduction: *DATRD2* in *NRCVAX96* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *NRCVAX96* and *SHELXL97* (Sheldrick, 1997b); molecular graphics: *NRCVAX96*, *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 1999); software used to prepare material for publication: *NRCVAX96*, *SHELXL97* and *WORDPERFECT* macro PREP8 (Ferguson, 1998)

6-Amino-5-*N*-acetyl-N-(β-*D*-3,4,6-tri-*O*-acetylglucopyranosyl)amino- 2,4-dioxo-1,2,3,4-tetrahydro-3-methyl-pyrimidine, water solvent

Crystal data

$C_{19}H_{26}N_4O_{11}·H_2O$	$V = 2462.0 (4)$ Å^3
$M_r = 504.45$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$
$a = 14.3951 (11)$ Å	$\mu = 0.11$ mm^{-1}
$b = 8.9771 (9)$ Å	$T = 294 (1)$ K
$c = 19.052 (2)$ Å	$0.40 \times 0.28 \times 0.17$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.089$
Absorption correction: none	3 standard reflections
4371 measured reflections	every 180 min
2495 independent reflections	intensity decay: no decay, variation 1.0%
1569 reflections with $I > 2\sigma(I)$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$	2 restraints
$wR(F^2) = 0.148$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$\Delta\rho_{max} = 0.24$ e Å^{-3}

2495 reflections

327 parameters

$\Delta\rho_{min} = -0.20$ e Å^{-3}

6-Acetamido-5-*N*-acetyl-N-(β-*D*-2,3,4,6-tetra-*O*-acetylglucopyranosyl)amino- 2,4-dioxo-1,2,3,4-tetrahydro-3-methyl-pyrimidine

Crystal data

$C_{23}H_{30}N_4O_{13}$

$M_r = 570.51$

Orthorhombic, $P2_12_12_1$

$a = 9.0315$ (8) Å

$b = 17.0918$ (13) Å

$c = 18.1487$ (13) Å

$V = 2801.5$ (4) Å^3

$Z = 4$

Mo $K\alpha$

$\mu = 0.11$ mm^{-1}

$T = 294$ (1) K

$0.41 \times 0.41 \times 0.10$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer

Absorption correction: none

5189 measured reflections

2942 independent reflections

1840 reflections with $I > 2\sigma(I)$

$R_{int} = 0.032$

3 standard reflections

every 180 min

intensity decay: no decay, variation 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.099$

$S = 0.99$

2942 reflections

361 parameters

H-atom parameters constrained

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

References

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Scheme 1
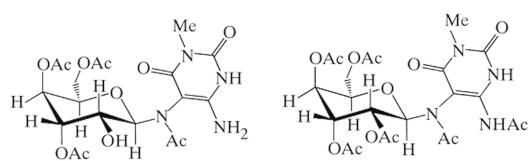
supplementary materials

6-Amino-5-*N*-acetyl-N-(β-*D*-3,4,6-tri-*O*-acetylglucopyranosyl)amino- 2,4-dioxo-1,2,3,4-tetrahydro-3-methyl-pyrimidine, water solvent

Crystal data

$C_{19}H_{26}N_4O_{11} \cdot H_2O$	? #Insert any comments here.
$M_r = 504.45$	$D_x = 1.361$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.3951$ (11) Å	Cell parameters from 25 reflections
$b = 8.9771$ (9) Å	$\theta = 9.7–13.8°$
$c = 19.052$ (2) Å	$\mu = 0.11$ mm^{-1}
$V = 2462.0$ (4) Å^3	$T = 294$ (1) K
$Z = 4$	Block, colorless
$F_{000} = 1064$	$0.40 \times 0.28 \times 0.17$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.089$
Radiation source: X-ray tube	$\theta_{max} = 25.1°$
Monochromator: graphite	$\theta_{min} = 2.1°$
$T = 294(1)$ K	$h = -17 \rightarrow 17$
$\theta/2\theta$ scans	$k = -10 \rightarrow 10$
Absorption correction: none	$l = -22 \rightarrow 22$
4371 measured reflections	3 standard reflections
2495 independent reflections	every 180 min
1569 reflections with $I > 2\sigma(I)$	intensity decay: no decay, variation 1.0%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.006$
2495 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
327 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

supplementary materials

Special details

Experimental. ? #Insert any special details here.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
N1	0.2954 (3)	0.0255 (5)	0.3870 (2)	0.0555 (12)	
H1	0.3412	0.0240	0.4159	0.067*	
C2	0.2250 (4)	0.1236 (7)	0.4001 (3)	0.0601 (15)	
O2	0.2267 (4)	0.2015 (5)	0.4528 (2)	0.0790 (13)	
N3	0.1574 (3)	0.1311 (5)	0.3499 (2)	0.0588 (12)	
C3	0.0823 (5)	0.2393 (8)	0.3604 (4)	0.088 (2)	
H3A	0.0530	0.2601	0.3162	0.133*	0.50
H3B	0.1074	0.3298	0.3794	0.133*	0.50
H3C	0.0373	0.1990	0.3924	0.133*	0.50
H3D	0.0789	0.2658	0.4091	0.133*	0.50
H3E	0.0244	0.1961	0.3459	0.133*	0.50
H3F	0.0945	0.3269	0.3330	0.133*	0.50
C4	0.1563 (4)	0.0409 (7)	0.2894 (3)	0.0538 (14)	
O4	0.0906 (3)	0.0555 (5)	0.2484 (2)	0.0708 (11)	
N5	0.2257 (3)	−0.1637 (5)	0.2239 (2)	0.0461 (10)	
C5	0.2292 (3)	−0.0638 (6)	0.2813 (2)	0.0432 (12)	
C51	0.1755 (4)	−0.2948 (7)	0.2267 (3)	0.0574 (14)	
O51	0.1742 (3)	−0.3797 (5)	0.1768 (2)	0.0761 (13)	
C52	0.1244 (5)	−0.3270 (8)	0.2926 (3)	0.081 (2)	
H52A	0.0943	−0.4221	0.2889	0.121*	
H52B	0.0787	−0.2510	0.3005	0.121*	
H52C	0.1673	−0.3288	0.3312	0.121*	
C6	0.2988 (3)	−0.0709 (6)	0.3312 (3)	0.0476 (13)	
N6	0.3695 (3)	−0.1666 (5)	0.3278 (2)	0.0599 (13)	
H6A	0.4113	−0.1667	0.3601	0.072*	
H6B	0.3732	−0.2283	0.2934	0.072*	
C1'	0.2737 (4)	−0.1298 (6)	0.1602 (3)	0.0452 (12)	
H1'	0.2478	−0.1915	0.1225	0.054*	
C2'	0.2655 (4)	0.0323 (6)	0.1390 (3)	0.0478 (13)	
H2'a	0.2846	0.0952	0.1785	0.057*	
O2'	0.1712 (3)	0.0641 (6)	0.12180 (19)	0.0690 (12)	

H2'b	0.1419	0.0803	0.1579	0.103*
C3'	0.3248 (4)	0.0682 (5)	0.0762 (2)	0.0438 (12)
H3'	0.2963	0.0263	0.0338	0.053*
O3'	0.3267 (3)	0.2287 (4)	0.07108 (18)	0.0583 (10)
C31'	0.3139 (4)	0.2928 (7)	0.0095 (4)	0.0666 (17)
O32'	0.3068 (5)	0.2255 (6)	−0.0434 (3)	0.118 (2)
C32'	0.3170 (6)	0.4585 (7)	0.0165 (4)	0.095 (2)
H32A	0.3805	0.4909	0.0184	0.142*
H32B	0.2856	0.4878	0.0587	0.142*
H32C	0.2869	0.5033	−0.0232	0.142*
C4'	0.4224 (4)	0.0074 (6)	0.0844 (2)	0.0445 (12)
H4'	0.4578	0.0670	0.1183	0.053*
O4'	0.4674 (2)	0.0096 (4)	0.01555 (17)	0.0511 (9)
C41'	0.5227 (4)	0.1232 (7)	−0.0010 (3)	0.0595 (15)
O41'	0.5376 (4)	0.2232 (6)	0.0393 (2)	0.0967 (17)
C42'	0.5580 (5)	0.1130 (9)	−0.0741 (3)	0.093 (2)
H42A	0.5840	0.2071	−0.0878	0.139*
H42B	0.5078	0.0879	−0.1051	0.139*
H42C	0.6050	0.0374	−0.0767	0.139*
C5'	0.4208 (4)	−0.1551 (6)	0.1062 (2)	0.0459 (12)
H5'	0.3886	−0.2120	0.0697	0.055*
O6'	0.3700 (2)	−0.1692 (4)	0.16960 (17)	0.0454 (8)
C6'	0.5152 (4)	−0.2217 (7)	0.1166 (3)	0.0611 (15)
H6C	0.5090	−0.3216	0.1355	0.073*
H6D	0.5468	−0.2285	0.0718	0.073*
O61'	0.5691 (3)	−0.1324 (5)	0.1639 (2)	0.0659 (11)
C61'	0.5809 (5)	−0.1813 (7)	0.2304 (4)	0.0695 (17)
O62'	0.5514 (3)	−0.2980 (5)	0.2503 (2)	0.0856 (14)
C62'	0.6337 (7)	−0.0744 (9)	0.2719 (4)	0.130 (4)
H62A	0.5924	0.0001	0.2901	0.195*
H62B	0.6797	−0.0278	0.2427	0.195*
H62C	0.6637	−0.1250	0.3100	0.195*
O1	0.0734 (4)	−0.0192 (7)	−0.0008 (3)	0.0905 (15)
H1A	0.063	0.080	0.003	0.136*
H1B	0.116	−0.023	0.034	0.136*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.067 (3)	0.061 (3)	0.037 (2)	−0.015 (3)	−0.010 (2)	−0.005 (2)
C2	0.075 (4)	0.047 (3)	0.058 (4)	−0.011 (3)	0.010 (3)	0.003 (3)
O2	0.123 (4)	0.065 (3)	0.049 (2)	−0.008 (3)	0.005 (3)	−0.020 (2)
N3	0.071 (3)	0.055 (3)	0.051 (3)	0.003 (3)	0.010 (2)	−0.004 (2)
C3	0.112 (5)	0.074 (4)	0.079 (5)	0.028 (5)	0.020 (4)	−0.004 (4)
C4	0.064 (3)	0.061 (3)	0.037 (3)	−0.001 (3)	0.004 (3)	0.005 (3)
O4	0.060 (2)	0.098 (3)	0.054 (2)	0.021 (2)	−0.005 (2)	−0.007 (2)
N5	0.049 (2)	0.044 (2)	0.045 (2)	−0.004 (2)	−0.002 (2)	−0.002 (2)
C5	0.051 (3)	0.048 (3)	0.030 (3)	−0.004 (3)	−0.003 (2)	0.000 (2)

C51	0.058 (3)	0.061 (3)	0.053 (3)	−0.012 (3)	−0.005 (3)	−0.006 (3)
O51	0.095 (3)	0.071 (3)	0.062 (3)	−0.029 (3)	−0.002 (3)	−0.016 (2)
C52	0.084 (4)	0.083 (5)	0.076 (4)	−0.035 (4)	0.010 (4)	0.002 (4)
C6	0.055 (3)	0.048 (3)	0.040 (3)	−0.009 (3)	0.001 (3)	0.006 (3)
N6	0.064 (3)	0.077 (3)	0.039 (2)	0.007 (3)	−0.014 (2)	0.000 (3)
C1'	0.047 (3)	0.044 (3)	0.045 (3)	−0.002 (3)	−0.007 (2)	0.001 (3)
C2'	0.055 (3)	0.043 (3)	0.045 (3)	0.009 (3)	−0.007 (2)	−0.001 (2)
O2'	0.063 (2)	0.090 (3)	0.053 (2)	0.026 (2)	−0.005 (2)	0.012 (2)
C3'	0.063 (3)	0.037 (3)	0.031 (3)	0.003 (3)	−0.004 (3)	0.005 (2)
O3'	0.089 (3)	0.045 (2)	0.041 (2)	0.006 (2)	−0.005 (2)	0.0064 (18)
C31'	0.077 (4)	0.062 (4)	0.061 (4)	−0.005 (3)	−0.018 (3)	0.025 (4)
O32'	0.209 (7)	0.093 (4)	0.051 (3)	−0.030 (5)	−0.045 (4)	0.019 (3)
C32'	0.126 (6)	0.058 (4)	0.100 (6)	0.013 (4)	0.006 (5)	0.031 (4)
C4'	0.060 (3)	0.044 (3)	0.029 (2)	0.000 (3)	−0.002 (2)	−0.003 (2)
O4'	0.067 (2)	0.050 (2)	0.0365 (19)	−0.0085 (19)	0.0072 (17)	−0.0055 (17)
C41'	0.072 (4)	0.066 (4)	0.040 (3)	−0.017 (3)	−0.002 (3)	0.004 (3)
O41'	0.142 (4)	0.089 (3)	0.059 (3)	−0.061 (4)	0.010 (3)	−0.013 (3)
C42'	0.103 (5)	0.113 (6)	0.063 (4)	−0.032 (5)	0.032 (4)	0.004 (4)
C5'	0.059 (3)	0.050 (3)	0.029 (3)	0.005 (3)	0.003 (2)	−0.003 (2)
O6'	0.0514 (19)	0.0440 (19)	0.0408 (19)	0.0043 (17)	−0.0069 (16)	0.0058 (16)
C6'	0.066 (3)	0.061 (3)	0.056 (4)	0.018 (3)	0.004 (3)	0.006 (3)
O61'	0.061 (2)	0.073 (3)	0.064 (3)	0.005 (2)	−0.011 (2)	0.017 (2)
C61'	0.075 (4)	0.055 (4)	0.078 (5)	0.013 (4)	−0.020 (4)	0.003 (4)
O62'	0.114 (3)	0.072 (3)	0.071 (3)	−0.008 (3)	−0.014 (3)	0.023 (3)
C62'	0.165 (8)	0.079 (5)	0.146 (8)	−0.014 (6)	−0.104 (7)	0.008 (5)
O1	0.091 (3)	0.105 (4)	0.075 (3)	0.003 (4)	0.007 (3)	−0.015 (3)

Geometric parameters (Å, °)

N1—C2	1.366 (7)	C2'—C3'	1.505 (7)
N1—C6	1.370 (7)	C3'—O3'	1.444 (6)
C2—O2	1.223 (7)	C3'—C4'	1.516 (7)
C2—N3	1.366 (7)	O3'—C31'	1.320 (7)
N3—C4	1.409 (7)	C31'—O32'	1.180 (8)
N3—C3	1.467 (7)	C31'—C32'	1.494 (10)
C4—O4	1.234 (6)	C4'—O4'	1.463 (6)
C4—C5	1.417 (7)	C4'—C5'	1.517 (7)
N5—C51	1.383 (7)	O4'—C41'	1.331 (6)
N5—C5	1.416 (6)	C41'—O41'	1.201 (7)
N5—C1'	1.429 (6)	C41'—C42'	1.486 (8)
C5—C6	1.383 (7)	C5'—O6'	1.417 (5)
C51—O51	1.218 (6)	C5'—C6'	1.499 (7)
C51—C52	1.484 (8)	C6'—O61'	1.434 (6)
C6—N6	1.333 (6)	O61'—C61'	1.351 (7)
C1'—O6'	1.442 (6)	C61'—O62'	1.193 (8)
C1'—C2'	1.515 (7)	C61'—C62'	1.456 (9)
C2'—O2'	1.425 (6)		
C2—N1—C6	125.2 (5)	C3'—C2'—C1'	111.9 (5)
O2—C2—N3	124.1 (6)	O3'—C3'—C2'	106.1 (4)

O2—C2—N1	120.3 (6)	O3'—C3'—C4'	110.3 (5)
N3—C2—N1	115.6 (5)	C2'—C3'—C4'	111.5 (4)
C2—N3—C4	123.5 (5)	C31'—O3'—C3'	119.5 (5)
C2—N3—C3	117.6 (5)	O32'—C31'—O3'	123.3 (6)
C4—N3—C3	118.9 (5)	O32'—C31'—C32'	126.1 (7)
O4—C4—N3	117.7 (5)	O3'—C31'—C32'	110.5 (7)
O4—C4—C5	124.7 (5)	O4'—C4'—C3'	108.2 (4)
N3—C4—C5	117.6 (5)	O4'—C4'—C5'	105.4 (4)
C51—N5—C5	121.9 (4)	C3'—C4'—C5'	111.1 (5)
C51—N5—C1'	117.8 (4)	C41'—O4'—C4'	119.2 (4)
C5—N5—C1'	120.3 (4)	O41'—C41'—O4'	121.9 (5)
C6—C5—C4	119.5 (5)	O41'—C41'—C42'	125.7 (6)
C6—C5—N5	121.9 (5)	O4'—C41'—C42'	112.3 (5)
C4—C5—N5	118.6 (4)	O6'—C5'—C6'	108.6 (4)
O51—C51—N5	120.7 (5)	O6'—C5'—C4'	109.1 (4)
O51—C51—C52	122.1 (5)	C6'—C5'—C4'	113.9 (5)
N5—C51—C52	117.2 (5)	O6'—C5'—H5'	108.3
N6—C6—N1	118.2 (5)	C6'—C5'—H5'	108.3
N6—C6—C5	123.3 (5)	C4'—C5'—H5'	108.3
N1—C6—C5	118.5 (5)	C5'—O6'—C1'	111.6 (4)
N5—C1'—O6'	107.9 (4)	O61'—C6'—C5'	110.5 (4)
N5—C1'—C2'	113.1 (5)	C61'—O61'—C6'	118.4 (5)
O6'—C1'—C2'	110.1 (4)	O62'—C61'—O61'	122.6 (6)
O2'—C2'—C3'	108.3 (4)	O62'—C61'—C62'	126.3 (7)
O2'—C2'—C1'	109.2 (5)	O61'—C61'—C62'	111.1 (6)
C6—N1—C2—O2	177.4 (5)	O6'—C1'—C2'—O2'	173.1 (4)
C6—N1—C2—N3	−5.2 (7)	N5—C1'—C2'—C3'	174.0 (4)
O2—C2—N3—C4	179.9 (5)	O6'—C1'—C2'—C3'	53.2 (6)
N1—C2—N3—C4	2.5 (8)	O2'—C2'—C3'—O3'	71.8 (5)
O2—C2—N3—C3	−0.2 (8)	C1'—C2'—C3'—O3'	−167.8 (4)
N1—C2—N3—C3	−177.6 (5)	O2'—C2'—C3'—C4'	−168.0 (5)
C2—N3—C4—O4	178.5 (5)	C1'—C2'—C3'—C4'	−47.6 (6)
C3—N3—C4—O4	−1.4 (8)	C2'—C3'—O3'—C31'	−134.4 (5)
C2—N3—C4—C5	0.7 (8)	C4'—C3'—O3'—C31'	104.7 (6)
C3—N3—C4—C5	−179.2 (5)	C3'—O3'—C31'—O32'	−5.1 (10)
O4—C4—C5—C6	−179.3 (5)	C3'—O3'—C31'—C32'	179.0 (6)
N3—C4—C5—C6	−1.6 (7)	O3'—C3'—C4'—O4'	−77.6 (5)
O4—C4—C5—N5	−2.6 (8)	C2'—C3'—C4'—O4'	164.7 (4)
N3—C4—C5—N5	175.1 (5)	O3'—C3'—C4'—C5'	167.1 (4)
C51—N5—C5—C6	92.7 (6)	C2'—C3'—C4'—C5'	49.4 (6)
C1'—N5—C5—C6	−88.2 (6)	C3'—C4'—O4'—C41'	97.0 (5)
C51—N5—C5—C4	−84.0 (6)	C5'—C4'—O4'—C41'	−144.1 (5)
C1'—N5—C5—C4	95.2 (6)	C4'—O4'—C41'—O41'	0.9 (8)
C5—N5—C51—O51	−179.3 (5)	C4'—O4'—C41'—C42'	−176.5 (5)
C1'—N5—C51—O51	1.5 (8)	O4'—C4'—C5'—O6'	−174.3 (3)
C5—N5—C51—C52	0.4 (7)	C3'—C4'—C5'—O6'	−57.3 (5)
C1'—N5—C51—C52	−178.8 (5)	O4'—C4'—C5'—C6'	64.1 (5)
C2—N1—C6—N6	−175.9 (5)	C3'—C4'—C5'—C6'	−178.9 (4)
C2—N1—C6—C5	4.3 (7)	C6'—C5'—O6'—C1'	−170.5 (4)

C4—C5—C6—N6	179.6 (5)	C4'—C5'—O6'—C1'	64.7 (5)
N5—C5—C6—N6	3.0 (8)	N5—C1'—O6'—C5'	173.3 (4)
C4—C5—C6—N1	−0.7 (7)	C2'—C1'—O6'—C5'	−62.8 (5)
N5—C5—C6—N1	−177.3 (4)	O6'—C5'—C6'—O61'	−69.0 (5)
C51—N5—C1'—O6'	−100.0 (5)	C4'—C5'—C6'—O61'	52.9 (6)
C5—N5—C1'—O6'	80.9 (6)	C5'—C6'—O61'—C61'	104.1 (5)
C51—N5—C1'—C2'	138.0 (5)	C6'—O61'—C61'—O62'	2.9 (9)
C5—N5—C1'—C2'	−41.1 (6)	C6'—O61'—C61'—C62'	−177.5 (6)
N5—C1'—C2'—O2'	−66.2 (5)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N6—H6B⋯O6'	0.86	2.48	3.015 (5)	126
O2'—H2'b⋯O4	0.82	1.89	2.678 (5)	161
O1—H1B⋯O2'	0.90	2.01	2.828 (7)	149
O1—H1A⋯O41[i]	0.90	1.97	2.804 (8)	152
N1—H1⋯O1[ii]	0.86	2.01	2.854 (7)	167
N6—H6A⋯O41[iii]	0.86	2.29	3.029 (6)	145

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

6-Acetamido-5-*N*-acetyl-N-(β-*D*-2,3,4,6-tetra-*O*-acetylglucopyranosyl)amino- 2,4-dioxo-1,2,3,4-tetrahydro-3-methyl-pyrimidine

Crystal data

$C_{23}H_{30}N_4O_{13}$	? #Insert any comments here.
$M_r = 570.51$	$D_x = 1.353$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.0315$ (8) Å	Cell parameters from 25 reflections
$b = 17.0918$ (13) Å	$\theta = 5.6–11.3°$
$c = 18.1487$ (13) Å	$\mu = 0.11$ mm^{-1}
$V = 2801.5$ (4) Å^3	$T = 294$ (1) K
$Z = 4$	Lath, colorless
$F_{000} = 1200$	$0.41 \times 0.41 \times 0.10$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.032$
Radiation source: X-ray tube	$\theta_{max} = 25.5°$
Monochromator: graphite	$\theta_{min} = 2.2°$
$T = 294(1)$ K	$h = −10 \rightarrow 10$
$\theta/2\theta$ scans	$k = −20 \rightarrow 20$
Absorption correction: none	$l = −21 \rightarrow 21$
5189 measured reflections	3 standard reflections
2942 independent reflections	every 180 min

1840 reflections with $I > 2\sigma(I)$

intensity decay: no decay, variation 1.0%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.099$

$S = 0.99$

2942 reflections

361 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.17$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL97,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0109 (10)

Special details

Experimental. ? #Insert any special details here.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
N1	0.4235 (3)	0.4812 (2)	0.40846 (17)	0.0661 (9)	
C2	0.2851 (4)	0.5070 (3)	0.4266 (2)	0.0750 (13)	
N3	0.2791 (3)	0.56059 (19)	0.48267 (17)	0.0534 (8)	
C4	0.4015 (4)	0.5860 (2)	0.52290 (19)	0.0482 (9)	
C5	0.5420 (4)	0.54954 (19)	0.50407 (18)	0.0435 (8)	
C6	0.5499 (4)	0.5001 (2)	0.44572 (18)	0.0467 (8)	
O2	0.1771 (3)	0.4840 (3)	0.3943 (2)	0.1334 (18)	
C31	0.1317 (4)	0.5900 (3)	0.5035 (2)	0.0692 (12)	
O4	0.3878 (3)	0.63725 (15)	0.56942 (14)	0.0603 (7)	
N5	0.6695 (3)	0.57136 (15)	0.54482 (14)	0.0427 (7)	
C51	0.7381 (4)	0.6433 (2)	0.5339 (2)	0.0518 (9)	
O52	0.8410 (3)	0.66364 (16)	0.57152 (17)	0.0747 (8)	
C52	0.6801 (5)	0.6914 (2)	0.4713 (2)	0.0727 (12)	
N6	0.6791 (3)	0.46520 (17)	0.42376 (15)	0.0492 (7)	
C61	0.7080 (4)	0.4321 (2)	0.35586 (19)	0.0506 (9)	
O62	0.6173 (3)	0.43281 (18)	0.30634 (13)	0.0719 (8)	
C62	0.8579 (4)	0.3971 (2)	0.3488 (2)	0.0663 (11)	
C1'	0.7296 (3)	0.52097 (18)	0.60133 (17)	0.0404 (7)	
C2'	0.6158 (3)	0.47136 (19)	0.64087 (17)	0.0415 (8)	
O21'	0.5185 (3)	0.52179 (14)	0.68201 (12)	0.0521 (6)	
C21'	0.3693 (4)	0.5093 (3)	0.6752 (2)	0.0609 (10)	
O22'	0.3186 (3)	0.46071 (19)	0.63625 (17)	0.0779 (9)	
C22'	0.2881 (4)	0.5659 (3)	0.7219 (2)	0.0893 (15)	

C3'	0.6923 (4)	0.4181 (2)	0.69545 (17)	0.0460 (8)	
O31'	0.5845 (3)	0.36388 (14)	0.72332 (13)	0.0594 (7)	
C31'	0.5627 (5)	0.3584 (3)	0.7962 (2)	0.0692 (11)	
O32'	0.6282 (5)	0.3986 (2)	0.83938 (15)	0.1016 (12)	
C32'	0.4511 (7)	0.2975 (3)	0.8146 (3)	0.114 (2)	
C4'	0.8141 (4)	0.3712 (2)	0.65923 (18)	0.0498 (9)	
O41'	0.9026 (3)	0.33449 (14)	0.71608 (13)	0.0597 (7)	
C41'	0.9001 (6)	0.2557 (2)	0.7217 (3)	0.0733 (12)	
O42'	0.8301 (5)	0.21538 (19)	0.6819 (2)	0.1273 (16)	
C42'	0.9988 (6)	0.2300 (3)	0.7826 (2)	0.0908 (15)	
C5'	0.9177 (4)	0.4236 (2)	0.61575 (18)	0.0468 (8)	
C6'	1.0332 (4)	0.3796 (2)	0.5728 (2)	0.0598 (10)	
O61'	0.9636 (3)	0.32346 (15)	0.52550 (15)	0.0661 (7)	
C61'	1.0092 (6)	0.2501 (3)	0.5281 (3)	0.0851 (15)	
O62'	1.1020 (5)	0.2282 (2)	0.5706 (3)	0.1466 (19)	
C62'	0.9317 (2)	0.19943 (11)	0.47592 (11)	0.144 (3)	
O6'	0.8316 (2)	0.46883 (11)	0.56494 (11)	0.0453 (6)	
H1	0.4316	0.4508	0.3709	0.079*	
H31A	0.1414	0.6268	0.5432	0.104*	0.50
H31B	0.0707	0.5470	0.5191	0.104*	0.50
H31C	0.0868	0.6153	0.4619	0.104*	0.50
H31D	0.0578	0.5659	0.4730	0.104*	0.50
H31E	0.1286	0.6457	0.4971	0.104*	0.50
H31F	0.1125	0.5775	0.5542	0.104*	0.50
H41A	0.7440	0.7355	0.4634	0.109*	
H41B	0.5822	0.7095	0.4828	0.109*	
H41C	0.6769	0.6601	0.4274	0.109*	
H6	0.7496	0.4638	0.4556	0.059*	
H62A	0.9104	0.4030	0.3945	0.099*	0.50
H62B	0.9112	0.4231	0.3102	0.099*	0.50
H62C	0.8489	0.3425	0.3373	0.099*	0.50
H62D	0.8700	0.3761	0.3002	0.099*	0.50
H62E	0.8691	0.3560	0.3844	0.099*	0.50
H62F	0.9314	0.4366	0.3574	0.099*	0.50
H1'	0.7835	0.5527	0.6374	0.048*	
H2'	0.5589	0.4404	0.6053	0.050*	
H22A	0.3576	0.5984	0.7477	0.134*	0.50
H22B	0.2284	0.5380	0.7569	0.134*	0.50
H22C	0.2257	0.5978	0.6915	0.134*	0.50
H22D	0.1835	0.5577	0.7164	0.134*	0.50
H22E	0.3128	0.6182	0.7071	0.134*	0.50
H22F	0.3154	0.5583	0.7726	0.134*	0.50
H3'	0.7333	0.4491	0.7361	0.055*	
H32A	0.4161	0.2735	0.7701	0.171*	0.50
H32B	0.3695	0.3212	0.8401	0.171*	0.50
H32C	0.4956	0.2585	0.8456	0.171*	0.50
H32D	0.4381	0.2953	0.8671	0.171*	0.50
H32E	0.4846	0.2476	0.7971	0.171*	0.50
H32F	0.3585	0.3103	0.7916	0.171*	0.50

H4'	0.7713	0.3312	0.6269	0.060*	
H42A	1.0705	0.1936	0.7640	0.136*	
H42B	0.9408	0.2053	0.8203	0.136*	
H42C	1.0489	0.2747	0.8029	0.136*	
H5'	0.9675	0.4593	0.6500	0.056*	
H6'A	1.0911	0.4159	0.5436	0.072*	
H6'B	1.0996	0.3530	0.6066	0.072*	
H62G	0.8621	0.2299	0.4481	0.215*	0.50
H62H	0.8801	0.1591	0.5023	0.215*	0.50
H62I	1.0022	0.1760	0.4430	0.215*	0.50
H62J	0.9675	0.1468	0.4809	0.215*	0.50
H62K	0.9495	0.2175	0.4266	0.215*	0.50
H62L	0.8274	0.2007	0.4859	0.215*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0440 (18)	0.101 (3)	0.0534 (17)	−0.0024 (19)	−0.0070 (14)	−0.0234 (18)
C2	0.040 (2)	0.113 (4)	0.072 (3)	0.001 (2)	−0.012 (2)	−0.016 (3)
N3	0.0370 (16)	0.065 (2)	0.0583 (18)	0.0021 (15)	−0.0056 (14)	0.0009 (17)
C4	0.0427 (19)	0.050 (2)	0.052 (2)	0.0010 (18)	−0.0027 (18)	0.0081 (19)
C5	0.0373 (18)	0.0440 (19)	0.0493 (19)	−0.0015 (16)	−0.0060 (16)	−0.0011 (16)
C6	0.042 (2)	0.053 (2)	0.0455 (19)	−0.0049 (18)	−0.0035 (16)	0.0038 (18)
O2	0.0493 (17)	0.230 (5)	0.121 (3)	0.003 (3)	−0.0274 (19)	−0.085 (3)
C31	0.041 (2)	0.081 (3)	0.086 (3)	0.005 (2)	−0.009 (2)	0.002 (3)
O4	0.0527 (15)	0.0555 (15)	0.0725 (16)	0.0126 (13)	−0.0044 (14)	−0.0118 (14)
N5	0.0370 (15)	0.0373 (15)	0.0539 (16)	−0.0031 (14)	−0.0067 (13)	−0.0006 (13)
C51	0.044 (2)	0.041 (2)	0.071 (2)	−0.0011 (18)	0.003 (2)	−0.0073 (19)
O52	0.0609 (17)	0.0623 (17)	0.101 (2)	−0.0217 (14)	−0.0150 (18)	−0.0073 (16)
C52	0.067 (3)	0.050 (2)	0.101 (3)	0.001 (2)	−0.003 (3)	0.016 (2)
N6	0.0392 (15)	0.0609 (18)	0.0477 (16)	−0.0007 (15)	−0.0001 (13)	−0.0043 (14)
C61	0.054 (2)	0.049 (2)	0.049 (2)	−0.012 (2)	0.0054 (19)	0.0000 (18)
O62	0.0692 (17)	0.098 (2)	0.0485 (14)	−0.0053 (18)	−0.0062 (14)	−0.0154 (15)
C62	0.065 (3)	0.074 (3)	0.060 (2)	0.002 (2)	0.016 (2)	−0.005 (2)
C1'	0.0349 (16)	0.0409 (17)	0.0453 (17)	0.0041 (16)	−0.0074 (15)	−0.0049 (15)
C2'	0.0369 (17)	0.0468 (19)	0.0407 (16)	−0.0017 (17)	−0.0030 (16)	−0.0081 (16)
O21'	0.0414 (13)	0.0653 (15)	0.0495 (13)	0.0064 (13)	0.0000 (11)	−0.0133 (12)
C21'	0.049 (2)	0.081 (3)	0.053 (2)	0.005 (2)	0.0010 (19)	0.001 (2)
O22'	0.0482 (16)	0.098 (2)	0.088 (2)	−0.0082 (17)	−0.0015 (15)	−0.0164 (19)
C22'	0.059 (2)	0.135 (4)	0.074 (3)	0.031 (3)	0.004 (2)	−0.022 (3)
C3'	0.047 (2)	0.0480 (19)	0.0429 (17)	−0.0029 (18)	−0.0026 (16)	−0.0040 (16)
O31'	0.0591 (15)	0.0671 (16)	0.0519 (15)	−0.0103 (14)	0.0021 (13)	0.0021 (13)
C31'	0.084 (3)	0.068 (3)	0.056 (3)	0.004 (3)	0.008 (2)	0.009 (2)
O32'	0.138 (3)	0.113 (3)	0.0528 (17)	−0.026 (3)	0.004 (2)	0.0017 (18)
C32'	0.127 (5)	0.111 (4)	0.104 (4)	−0.039 (4)	0.029 (4)	0.018 (3)
C4'	0.050 (2)	0.0481 (19)	0.0510 (19)	0.0038 (19)	−0.0115 (18)	−0.0015 (16)
O41'	0.0636 (16)	0.0589 (16)	0.0565 (14)	0.0119 (14)	−0.0178 (13)	0.0030 (12)
C41'	0.094 (3)	0.053 (2)	0.073 (3)	−0.001 (3)	−0.009 (3)	0.012 (2)

O42'	0.189 (4)	0.062 (2)	0.132 (3)	−0.033 (2)	−0.074 (3)	0.028 (2)
C42'	0.116 (4)	0.079 (3)	0.078 (3)	0.028 (3)	−0.024 (3)	0.020 (3)
C5'	0.0385 (18)	0.0459 (18)	0.056 (2)	0.0022 (18)	−0.0115 (17)	−0.0018 (17)
C6'	0.046 (2)	0.058 (2)	0.076 (2)	0.0071 (19)	−0.004 (2)	0.003 (2)
O61'	0.0706 (17)	0.0566 (15)	0.0711 (16)	0.0238 (15)	−0.0028 (15)	−0.0098 (13)
C61'	0.071 (3)	0.056 (3)	0.128 (4)	0.024 (2)	−0.001 (3)	0.007 (3)
O62'	0.117 (3)	0.070 (2)	0.253 (5)	0.029 (2)	−0.058 (4)	0.011 (3)
C62'	0.178 (7)	0.086 (4)	0.167 (6)	0.034 (5)	−0.020 (6)	−0.059 (4)
O6'	0.0406 (12)	0.0443 (12)	0.0510 (12)	0.0042 (11)	−0.0027 (11)	−0.0005 (11)

Geometric parameters (Å, °)

N1—C6	1.366 (4)	C2'—C3'	1.513 (4)
N1—C2	1.366 (5)	O21'—C21'	1.370 (5)
C2—O2	1.204 (5)	C21'—O22'	1.183 (5)
C2—N3	1.370 (6)	C21'—C22'	1.480 (6)
N3—C4	1.394 (4)	C3'—O31'	1.436 (4)
N3—C31	1.473 (5)	C3'—C4'	1.511 (5)
C4—O4	1.222 (4)	O31'—C31'	1.341 (5)
C4—C5	1.455 (5)	C31'—O32'	1.198 (5)
C5—C6	1.357 (4)	C31'—C32'	1.487 (6)
C5—N5	1.418 (4)	C4'—O41'	1.448 (4)
C6—N6	1.370 (4)	C4'—C5'	1.517 (5)
N5—C51	1.391 (4)	O41'—C41'	1.351 (5)
N5—C1'	1.445 (4)	C41'—O42'	1.181 (5)
C51—O52	1.204 (4)	C41'—C42'	1.486 (6)
C51—C52	1.498 (5)	C5'—O6'	1.432 (4)
N6—C61	1.381 (4)	C5'—C6'	1.504 (5)
C61—O62	1.217 (4)	C6'—O61'	1.433 (4)
C61—C62	1.485 (5)	O61'—C61'	1.321 (5)
C1'—O6'	1.442 (4)	C61'—O62'	1.199 (6)
C1'—C2'	1.514 (4)	C61'—C62'	1.462 (6)
C2'—O21'	1.439 (4)		
C6—N1—C2	124.7 (3)	O21'—C2'—C3'	107.4 (2)
O2—C2—N1	121.2 (4)	C1'—C2'—C3'	109.7 (3)
O2—C2—N3	123.2 (4)	C21'—O21'—C2'	117.4 (3)
N1—C2—N3	115.5 (3)	O22'—C21'—O21'	123.0 (4)
C2—N3—C4	124.5 (3)	O22'—C21'—C22'	127.5 (4)
C2—N3—C31	117.0 (3)	O21'—C21'—C22'	109.5 (4)
C4—N3—C31	118.4 (3)	O31'—C3'—C4'	107.7 (3)
O4—C4—N3	120.3 (3)	O31'—C3'—C2'	108.0 (3)
O4—C4—C5	123.9 (3)	C4'—C3'—C2'	111.5 (3)
N3—C4—C5	115.8 (3)	C31'—O31'—C3'	119.5 (3)
C6—C5—N5	121.9 (3)	O32'—C31'—O31'	122.2 (4)
C6—C5—C4	119.7 (3)	O32'—C31'—C32'	126.1 (4)
N5—C5—C4	118.2 (3)	O31'—C31'—C32'	111.7 (4)
C5—C6—N1	119.4 (3)	O41'—C4'—C3'	108.7 (3)
C5—C6—N6	122.9 (3)	O41'—C4'—C5'	106.6 (3)
N1—C6—N6	117.7 (3)	C3'—C4'—C5'	111.2 (3)

C51—N5—C5	121.3 (3)	C41'—O41'—C4'	118.5 (3)
C51—N5—C1'	117.4 (3)	O42'—C41'—O41'	123.0 (4)
C5—N5—C1'	121.2 (3)	O42'—C41'—C42'	127.1 (4)
O52—C51—N5	121.2 (4)	O41'—C41'—C42'	109.9 (4)
O52—C51—C52	122.8 (3)	O6'—C5'—C6'	108.3 (3)
N5—C51—C52	116.0 (3)	O6'—C5'—C4'	108.6 (2)
C6—N6—C61	126.8 (3)	C6'—C5'—C4'	113.6 (3)
O62—C61—N6	121.8 (3)	O61'—C6'—C5'	110.0 (3)
O62—C61—C62	123.7 (3)	C61'—O61'—C6'	118.5 (4)
N6—C61—C62	114.5 (3)	O62'—C61'—O61'	122.5 (5)
O6'—C1'—N5	106.5 (2)	O62'—C61'—C62'	124.5 (4)
O6'—C1'—C2'	107.8 (2)	O61'—C61'—C62'	113.0 (4)
N5—C1'—C2'	114.5 (3)	C5'—O6'—C1'	112.7 (2)
O21'—C2'—C1'	109.0 (2)		
C6—N1—C2—O2	−175.1 (5)	N5—C1'—C2'—O21'	−65.8 (3)
C6—N1—C2—N3	5.5 (7)	O6'—C1'—C2'—C3'	58.6 (3)
O2—C2—N3—C4	177.4 (5)	N5—C1'—C2'—C3'	176.9 (3)
N1—C2—N3—C4	−3.2 (6)	C1'—C2'—O21'—C21'	132.2 (3)
O2—C2—N3—C31	0.5 (7)	C3'—C2'—O21'—C21'	−109.1 (3)
N1—C2—N3—C31	179.8 (4)	C2'—O21'—C21'—O22'	−1.8 (6)
C2—N3—C4—O4	176.0 (4)	C2'—O21'—C21'—C22'	179.4 (3)
C31—N3—C4—O4	−7.1 (5)	O21'—C2'—C3'—O31'	70.5 (3)
C2—N3—C4—C5	−2.4 (5)	C1'—C2'—C3'—O31'	−171.2 (2)
C31—N3—C4—C5	174.6 (3)	O21'—C2'—C3'—C4'	−171.3 (3)
O4—C4—C5—C6	−172.0 (3)	C1'—C2'—C3'—C4'	−53.0 (4)
N3—C4—C5—C6	6.3 (5)	C4'—C3'—O31'—C31'	114.9 (3)
O4—C4—C5—N5	3.7 (5)	C2'—C3'—O31'—C31'	−124.5 (3)
N3—C4—C5—N5	−178.0 (3)	C3'—O31'—C31'—O32'	1.6 (6)
N5—C5—C6—N1	−180.0 (3)	C3'—O31'—C31'—C32'	−178.0 (3)
C4—C5—C6—N1	−4.4 (5)	O31'—C3'—C4'—O41'	−73.6 (3)
N5—C5—C6—N6	2.8 (5)	C2'—C3'—C4'—O41'	168.0 (3)
C4—C5—C6—N6	178.4 (3)	O31'—C3'—C4'—C5'	169.2 (2)
C2—N1—C6—C5	−1.8 (6)	C2'—C3'—C4'—C5'	50.9 (4)
C2—N1—C6—N6	175.6 (4)	C3'—C4'—O41'—C41'	113.4 (4)
C6—C5—N5—C51	101.2 (4)	C5'—C4'—O41'—C41'	−126.6 (4)
C4—C5—N5—C51	−74.4 (4)	C4'—O41'—C41'—O42'	0.7 (7)
C6—C5—N5—C1'	−81.2 (4)	C4'—O41'—C41'—C42'	179.5 (3)
C4—C5—N5—C1'	103.2 (4)	O41'—C4'—C5'—O6'	−172.7 (2)
C5—N5—C51—O52	175.6 (3)	C3'—C4'—C5'—O6'	−54.3 (3)
C1'—N5—C51—O52	−2.1 (5)	O41'—C4'—C5'—C6'	66.8 (3)
C5—N5—C51—C52	−6.7 (5)	C3'—C4'—C5'—C6'	−174.8 (3)
C1'—N5—C51—C52	175.6 (3)	O6'—C5'—C6'—O61'	−65.5 (3)
C5—C6—N6—C61	−161.2 (3)	C4'—C5'—C6'—O61'	55.2 (4)
N1—C6—N6—C61	21.6 (5)	C5'—C6'—O61'—C61'	−128.1 (4)
C6—N6—C61—O62	1.9 (6)	C6'—O61'—C61'—O62'	3.1 (7)
C6—N6—C61—C62	−178.8 (3)	C6'—O61'—C61'—C62'	−178.6 (3)
C51—N5—C1'—O6'	−94.4 (3)	C6'—C5'—O6'—C1'	−172.7 (3)
C5—N5—C1'—O6'	87.9 (3)	C4'—C5'—O6'—C1'	63.5 (3)
C51—N5—C1'—C2'	146.6 (3)	N5—C1'—O6'—C5'	170.6 (2)

C5—N5—C1'—C2'	−31.0 (4)	C2'—C1'—O6'—C5'	−66.1 (3)
O6'—C1'—C2'—O21'	176.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6···O6'	0.86	2.12	2.910 (4)	152
N1—H1···O62	0.86	2.07	2.680 (4)	127