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2-*N*,5′-Di-*O*-acetyl-2′,3′-*O*-isopropylideneguanosine monohydrate

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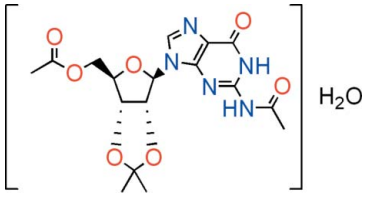
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.148; data-to-parameter ratio = 10.2.

The asymmetric unit of the title compound, $C_{17}H_{21}N_5O_7\cdot H_2O$, consists of two organic molecules (*A* and *B*) and two molecules of water. Both molecules show *R* configurations for all their chiral centres, and the furanose and dioxolane rings have envelope and twist conformations, respectively. The conformation of the nucleoside group is anti. The purine groups of the two molecules are almost parallel, with a dihedral angle between their mean planes of 4.90 (2)°. The molecules are stacked in the [010] direction, with alternating *A* and *B* molecules. Hydrogen bonds involving water molecules form an infinite one-dimensional chain, also along the crystallographic *b* axis. Hydrogen bonding between water molecules connects these chains, generating a double-sheet polymeric structure.

Related literature

For related literature, see: Allen *et al.* (1987); De Clercq & Field (2006); Mande *et al.* (1988, 1989); Sá & Meier (2006); Sá *et al.* (2002); Santaniello *et al.* (2005); Shi *et al.* (2001, 2003); Leitão *et al.* (2004).



Experimental

Crystal data

$C_{17}H_{21}N_5O_7\cdot H_2O$
M_r = 425.40
Triclinic, $P1$
a = 6.595 (1) Å
b = 9.688 (1) Å
c = 16.301 (1) Å
α = 72.72 (1)°
β = 89.68 (1)°
γ = 83.82 (1)°
V = 988.34 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
0.50 × 0.23 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
6620 measured reflections
5699 independent reflections
4093 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections
every 200 reflections
intensity decay: <1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.148
S = 1.03
5699 reflections
557 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O22	0.77 (6)	2.00 (6)	2.649 (4)	142 (5)
N11—H11···O122	0.89 (5)	2.01 (5)	2.690 (5)	133 (4)
N21—H21···O1W^{i}	0.89 (4)	1.88 (4)	2.757 (4)	168 (4)
N121—H121···O2W^{ii}	0.95 (5)	1.98 (5)	2.915 (5)	169 (4)
O2W—H2WA···N17	0.91	2.00	2.885 (4)	162
O1W—H1WA···N7	0.87	1.91	2.775 (4)	173
O2W—H2WB···O1W^{iii}	0.87	2.15	3.011 (5)	170

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *SET4* in *CAD-4 EXPRESS*; data reduction: *HELENA* (Spek, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2128).

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supplementary materials

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2-*N*,5'-Di-*O*-acetyl-2',3'-*O*-isopropylideneguanosine monohydrate

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Comment

Nucleosides and synthetically modified analogues participate in a variety of physiological processes (De Clercq & Field, 2006; Santaniello *et al.*, 2005) and are known to self-associate *via* hydrogen bonding and base stacking (Shi *et al.*, 2001). In particular, 2',3'-*O*-isopropylideneguanosine and derivatives are notable for their propensity to aggregate (Shi *et al.*, 2003; Mande *et al.*, 1988; Mande *et al.*, 1989). However, the crystal structures of N2-acetylated guanosines have not been reported so far. In continuation of our research on the chemistry of nucleosides (Sá *et al.*, 2002; Leitão *et al.*, 2004), we recently developed a simple and inexpensive method for the synthesis of 2',3'-*O*-isopropylidene-2-*N*-5'-*O*-diacetylguanosine (I) in good yield and high purity (Sá & Meier, 2006). We now report the crystal structure of this compound.

The asymmetric unit consists of two independent molecules of (I) (Fig. 1) and two molecules of water. Distinct intermolecular interactions (Table 2) and different conformational parameters (Table 1) between the independent molecules of (I) lead the asymmetric unit to be greater than expected. A similar feature was also observed in the crystal structure of 2',3'-*O*-isopropylideneguanosine (II) reported by Mande *et al.* (1989).

Bond lengths and angles are within the expected ranges (Allen *et al.*, 1987). Both molecules of (I) show *R* configuration for their chiral centers C1', C2', C3' and C4' in molecule A and C11', C12', C13' and C14' in molecule B. In molecule A the furanose ring adopts envelope conformation on C3' (pucker C3'-*exo*), where this atom is 0.421 (5) Å out of the least-squares plane defined by the remaining four atoms, with pseudorotation parameters P and τ_m of 20.6 (5)° and 27.6 (2)°. The dioxolane ring is twisted on O2—C2' bond and exhibits C30-*exo*–O2-*endo* type pucker with P = 112.7 (4)° and τ_m = 35.6 (2)°. Molecule B also shows the furanose ring as an envelope on C14' (pucker C14'-*exo*) with P = 233.3 (4)° and τ_m = 30.6 (2)°, where C14' is displaced of 0.431 (5) Å from the mean plane formed by the four other atoms. The dioxolane ring is twisted on C13'—O13 and exhibits C130-*exo*–O13-*endo* pucker type with pseudorotation parameters P = 355.8 (5)° and τ_m = 26.3 (2)°. In the *N*-acetylated groups, the conformation about the C4'—C5' bond is *gauche*–gauche with Φ_{OC} = 50.2 (5)° and Φ_{OO} = −69.7 (4)° for molecule A and about the C14'—C15' bond it is *gauche*-anti with Φ_{OC} = −75.4 (4)° and Φ_{OO} = 168.7 (3)° for molecule B. Similar conformations for these groups found in molecule A were reported for the crystal structure of compound (II) crystallized from Me_2SO by Mande *et al.* (1988), but they are significantly different from those determined for (II) crystallized from water/acetone (Mande *et al.*, 1989), where in both molecules the furanose rings are C1'-*endo*, the conformation around C4'—C5' bonds is anti–gauche and the dioxolane ring in molecule A (II) is C9-*endo*–O3'-*exo*.

The purine groups are essentially planar, but the deviation from planarity is slightly different in each independent molecule of (I). The r.m.s. deviations of 10 fitted atoms are 0.005 and 0.020 for molecules A and B, respectively. Despite the N—H···O intramolecular hydrogen bond (Table 2), the torsion angles N3—C2—N21—C22 of −179.0 (3)° and N13—C12—N121—C122 of 175.0 (3)° demonstrate that the terminal amide arms deviate distinctly from the correspondent purine mean plane, while the exocyclic O6 and O16 atoms are retained in their respective planes. The conformation of the nucleoside group is anti with torsion angles O1—C1'—N9—C4 of −140.1 (3)° [A] and O11—C11'—N19—C14 of

−178.9 (3)° [B]. These values are significantly different from those found in compound (II), with torsion angles of −94.1° (Mande *et al.*, 1988) and 74.1° and 77.5° (Mande *et al.*, 1989).

The purine groups of molecules A and B are almost parallel, with a dihedral angles between their mean planes of 4.90 (2)°. The molecules are stacked in the [010] direction, with intercalated A and B molecules. In addition, a very interesting packing take place through intermolecular interactions (Fig. 2). The water molecule O1W links A molecules and the water molecule O2W links B molecules, forming an infinite chain, also along the crystallographic *b* axis. The O2W—H2WB···O1W hydrogen bond between water molecules connects the two chains, thus building a double-sheet polymeric structure.

Experimental

Selective acetylation of 2',3'-*O*-isopropylideneguanosine employing a combination of acetic anhydride and recyclable 13X molecular sieves under heterogeneous conditions gave (I) in high purity (81% yield) according to the reported method (Sá & Meier, 2006). Slow crystallization from CH_2Cl_2/AcOEt/MeOH/hexane (1:18:2:1) furnished single crystals (mp 397–398 K), allowing structural elucidation by X-ray crystallographic technique. The absolute configuration for (I) was previously assigned based on ^{1}H– and ^{13}C-NMR shifts for the starting 2',3'-*O*-isopropylideneguanosine and on the homogeneity of the reaction product; in the absence of significant anomalous scattering, Friedel pairs were merged.

Refinement

H atoms attached to carbon atoms were positioned geometrically, with C—H = 0.96 (CH_3), 0.97 (CH_2) or 0.93 Å (CH_{Ar}), and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl groups. H atoms attached to N atoms were found in a difference Fourier map and refined freely. H atoms of the water molecules were also found in the difference map and treated as riding, with U_{iso}(H) = 1.2U_{eq}(O).

Figures

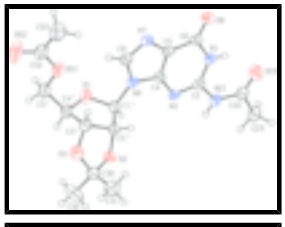


Fig. 1. The structures of the two indpendent molecules of (I) with the labeling scheme. Displacement ellipsoids are shown at the 40% probability level.

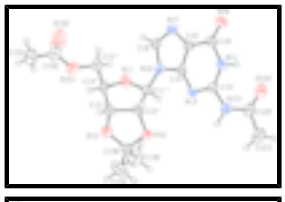
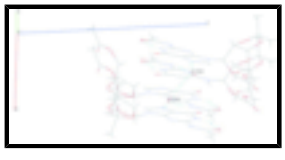


Fig. 2. Packing of (I) showing the molecules connected through hydrogen bonds (dashed lines) and stacked along the *b* axis.



2-*N*,5'-*O*-Diacetyl-2',3'-*O*-isopropylideneguanosine monohydrate

Crystal data

$C_{17}H_{21}N_5O_7 \cdot H_2O$	$Z = 2$
$M_r = 425.40$	$F_{000} = 448$
Triclinic, $P\overline{1}$	$D_x = 1.429$ Mg m^{-3}
Hall symbol: P -1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 6.595$ (1) Å	Cell parameters from 25 reflections
$b = 9.688$ (1) Å	$\theta = 5.1$–18.8º
$c = 16.301$ (1) Å	$\mu = 0.12$ mm^{-1}
$\alpha = 72.72$ (1)º	$T = 293$ (2) K
$\beta = 89.68$ (1)º	Prismatic, colourless
$\gamma = 83.82$ (1)º	0.50 × 0.23 × 0.16 mm
$V = 988.34$ (19) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.017$
Radiation source: fine-focus sealed tube	$\theta_{max} = 30.4$º
Monochromator: graphite	$\theta_{min} = 1.3$º
$T = 293$(2) K	$h = -9 \rightarrow 9$
ω/2θ scans	$k = -13 \rightarrow 13$
Absorption correction: none	$l = -22 \rightarrow 14$
6620 measured reflections	3 standard reflections
5699 independent reflections	every 200 reflections
4093 reflections with $I > 2\sigma(I)$	intensity decay: <1%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2 + 0.2093P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.148$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
5699 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
557 parameters	Extinction correction: none
3 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.5489 (4)	0.9264 (3)	0.7783 (2)	0.0340 (6)
C2	0.5637 (5)	0.9965 (3)	0.8396 (2)	0.0330 (6)
N3	0.5925 (4)	0.9319 (3)	0.92166 (18)	0.0333 (5)
C4	0.6092 (5)	0.7851 (3)	0.9397 (2)	0.0308 (6)
C5	0.5969 (5)	0.7023 (3)	0.8842 (2)	0.0315 (6)
C6	0.5635 (4)	0.7744 (3)	0.7943 (2)	0.0326 (6)
O6	0.5481 (4)	0.7239 (3)	0.73424 (16)	0.0429 (6)
N7	0.6223 (4)	0.5549 (3)	0.9301 (2)	0.0379 (6)
C8	0.6499 (6)	0.5519 (4)	1.0101 (2)	0.0396 (7)
H8	0.6718	0.4663	1.0554	0.048*
N9	0.6430 (4)	0.6879 (3)	1.02033 (18)	0.0356 (6)
C1'	0.6706 (5)	0.7256 (3)	1.0993 (2)	0.0378 (7)
H1'	0.7105	0.8243	1.0857	0.045*
C2'	0.4813 (6)	0.7141 (3)	1.1521 (2)	0.0390 (7)
H2'	0.3563	0.7205	1.1183	0.047*
C3'	0.5225 (6)	0.5712 (4)	1.2242 (2)	0.0440 (8)
H3'	0.4681	0.4908	1.2098	0.053*
O1	0.8251 (4)	0.6254 (3)	1.14928 (18)	0.0489 (6)
O2	0.4720 (5)	0.8171 (3)	1.19937 (16)	0.0483 (6)
O3	0.4292 (5)	0.5984 (3)	1.29675 (19)	0.0618 (8)
C4'	0.7534 (6)	0.5496 (4)	1.2324 (2)	0.0451 (8)
H4'	0.7951	0.5973	1.2739	0.054*
C5'	0.8544 (7)	0.3959 (4)	1.2589 (3)	0.0569 (10)
H5'1	1.0008	0.3949	1.2527	0.068*
H5'2	0.8273	0.3479	1.3186	0.068*
N21	0.5468 (5)	1.1468 (3)	0.8130 (2)	0.0399 (6)
C22	0.5137 (6)	1.2358 (4)	0.7312 (3)	0.0465 (8)
O22	0.4858 (6)	1.1924 (3)	0.6696 (2)	0.0707 (10)
C23	0.5148 (8)	1.3962 (4)	0.7225 (3)	0.0566 (10)
H23A	0.5388	1.4077	0.7780	0.085*
H23B	0.3853	1.4477	0.6992	0.085*
H23C	0.6209	1.4345	0.6847	0.085*
C30	0.3801 (7)	0.7531 (4)	1.2793 (3)	0.0522 (9)
C31	0.1567 (9)	0.7868 (7)	1.2703 (4)	0.0769 (14)
H31A	0.1211	0.8896	1.2587	0.115*
H31B	0.0954	0.7361	1.3226	0.115*
H31C	0.1079	0.7564	1.2237	0.115*
C32	0.4768 (12)	0.8041 (8)	1.3469 (4)	0.0900 (19)
H32A	0.4431	0.9072	1.3345	0.135*
H32B	0.6222	0.7819	1.3471	0.135*
H32C	0.4267	0.7556	1.4022	0.135*
O51	0.7718 (5)	0.3217 (3)	1.20395 (19)	0.0544 (7)
C52	0.8204 (8)	0.1780 (5)	1.2249 (3)	0.0665 (12)
O52	0.9266 (10)	0.1129 (5)	1.2856 (4)	0.132 (2)
C53	0.7288 (11)	0.1140 (6)	1.1641 (4)	0.0841 (17)

H53A	0.6539	0.1898	1.1194	0.126*
H53B	0.6381	0.0460	1.1941	0.126*
H53C	0.8348	0.0646	1.1392	0.126*
N11	0.1225 (4)	0.6227 (3)	0.9599 (2)	0.0398 (6)
C12	0.1310 (5)	0.5385 (4)	0.9062 (2)	0.0363 (7)
N13	0.1113 (4)	0.5873 (3)	0.82256 (18)	0.0355 (6)
C14	0.0864 (5)	0.7348 (3)	0.7941 (2)	0.0320 (6)
C15	0.0782 (5)	0.8324 (4)	0.8417 (2)	0.0351 (7)
C16	0.0982 (5)	0.7765 (4)	0.9338 (2)	0.0390 (7)
O16	0.1000 (4)	0.8424 (3)	0.98721 (18)	0.0520 (7)
N17	0.0603 (4)	0.9738 (3)	0.7872 (2)	0.0406 (6)
C18	0.0581 (5)	0.9593 (4)	0.7106 (3)	0.0414 (8)
H18	0.0497	1.0378	0.6608	0.050*
N19	0.0694 (4)	0.8164 (3)	0.70972 (18)	0.0354 (6)
C11'	0.0976 (5)	0.7588 (4)	0.6352 (2)	0.0372 (7)
H11'	0.2361	0.7093	0.6380	0.045*
C12'	−0.0567 (5)	0.6523 (4)	0.6323 (2)	0.0377 (7)
H12'	−0.1515	0.6411	0.6797	0.045*
O11	0.0717 (4)	0.8759 (3)	0.55897 (17)	0.0497 (6)
O12	0.0358 (5)	0.5154 (3)	0.62789 (18)	0.0500 (6)
O13	−0.0623 (6)	0.6514 (4)	0.4896 (2)	0.0706 (10)
C13'	−0.1672 (6)	0.7242 (4)	0.5448 (2)	0.0471 (8)
H13'	−0.3136	0.7144	0.5468	0.057*
C14'	−0.1235 (6)	0.8797 (4)	0.5190 (2)	0.0465 (8)
H14'	−0.1148	0.9166	0.4564	0.056*
C15'	−0.2766 (7)	0.9774 (5)	0.5506 (3)	0.0571 (10)
H15A	−0.3037	0.9310	0.6104	0.069*
H15B	−0.2215	1.0679	0.5465	0.069*
N121	0.1636 (5)	0.3876 (3)	0.9412 (2)	0.0449 (7)
C122	0.2035 (6)	0.3085 (5)	1.0258 (3)	0.0527 (9)
O122	0.2148 (6)	0.3671 (4)	1.0822 (2)	0.0726 (9)
C123	0.2362 (9)	0.1468 (5)	1.0408 (4)	0.0713 (14)
H12A	0.2212	0.1261	0.9873	0.107*
H12B	0.1374	0.1010	1.0802	0.107*
H12C	0.3710	0.1101	1.0647	0.107*
C130	0.0215 (7)	0.5106 (4)	0.5404 (3)	0.0501 (9)
C131	−0.1049 (13)	0.3942 (8)	0.5376 (4)	0.095 (2)
H13A	−0.0414	0.3021	0.5732	0.142*
H13B	−0.1169	0.3913	0.4795	0.142*
H13C	−0.2381	0.4138	0.5584	0.142*
C132	0.2314 (10)	0.4863 (8)	0.5091 (4)	0.0876 (19)
H13D	0.2943	0.3919	0.5415	0.131*
H13E	0.3111	0.5594	0.5163	0.131*
H13F	0.2240	0.4921	0.4493	0.131*
O151	−0.4605 (5)	1.0066 (4)	0.5013 (3)	0.0728 (10)
C152	−0.4991 (9)	1.1363 (6)	0.4447 (4)	0.0708 (13)
O152	−0.3852 (10)	1.2225 (6)	0.4326 (4)	0.137 (2)
C153	−0.7059 (10)	1.1552 (8)	0.4044 (5)	0.103 (2)
H15C	−0.7699	1.0678	0.4272	0.155*

H15D	−0.6945	1.1752	0.3433	0.155*
H15E	−0.7869	1.2349	0.4165	0.155*
O1W	0.6997 (5)	0.2679 (3)	0.9295 (2)	0.0657 (9)
H1WA	0.6671	0.3556	0.9329	0.079*
H1WB	0.7369	0.2105	0.9797	0.079*
O2W	0.0482 (5)	1.2583 (4)	0.8105 (2)	0.0660 (9)
H2WA	0.0698	1.1624	0.8136	0.079*
H2WB	−0.0548	1.2723	0.8414	0.079*
H1	0.530 (8)	0.980 (6)	0.733 (4)	0.064 (15)*
H11	0.138 (7)	0.576 (5)	1.016 (3)	0.055 (13)*
H21	0.580 (6)	1.182 (4)	0.855 (3)	0.030 (9)*
H121	0.143 (7)	0.339 (5)	0.900 (3)	0.048 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0362 (14)	0.0316 (13)	0.0335 (14)	−0.0039 (10)	0.0007 (11)	−0.0084 (11)
C2	0.0310 (15)	0.0286 (14)	0.0392 (17)	−0.0024 (11)	0.0035 (12)	−0.0104 (12)
N3	0.0397 (14)	0.0246 (12)	0.0364 (14)	−0.0035 (10)	0.0030 (11)	−0.0101 (10)
C4	0.0308 (14)	0.0284 (14)	0.0322 (15)	−0.0041 (11)	0.0031 (11)	−0.0073 (12)
C5	0.0302 (14)	0.0261 (13)	0.0400 (17)	−0.0039 (11)	0.0040 (12)	−0.0124 (12)
C6	0.0251 (14)	0.0344 (15)	0.0431 (17)	−0.0075 (11)	0.0077 (12)	−0.0174 (13)
O6	0.0470 (14)	0.0453 (14)	0.0432 (13)	−0.0093 (11)	0.0034 (11)	−0.0221 (11)
N7	0.0407 (15)	0.0271 (13)	0.0470 (16)	−0.0048 (11)	0.0042 (12)	−0.0125 (11)
C8	0.0500 (19)	0.0263 (14)	0.0424 (18)	−0.0051 (13)	0.0020 (14)	−0.0097 (13)
N9	0.0416 (15)	0.0255 (12)	0.0392 (14)	−0.0040 (10)	−0.0011 (11)	−0.0089 (11)
C1'	0.0502 (19)	0.0277 (14)	0.0358 (16)	−0.0042 (13)	−0.0027 (14)	−0.0098 (12)
C2'	0.0484 (19)	0.0326 (16)	0.0369 (16)	−0.0014 (13)	−0.0012 (14)	−0.0129 (13)
C3'	0.057 (2)	0.0300 (15)	0.0421 (18)	−0.0052 (14)	0.0023 (15)	−0.0058 (13)
O1	0.0426 (14)	0.0517 (15)	0.0448 (14)	−0.0016 (11)	−0.0063 (11)	−0.0041 (12)
O2	0.0747 (18)	0.0322 (12)	0.0386 (13)	−0.0031 (11)	0.0055 (12)	−0.0127 (10)
O3	0.085 (2)	0.0449 (15)	0.0465 (16)	0.0003 (14)	0.0218 (15)	−0.0028 (12)
C4'	0.058 (2)	0.0336 (17)	0.0380 (18)	−0.0025 (15)	−0.0061 (15)	−0.0031 (14)
C5'	0.068 (3)	0.0399 (19)	0.057 (2)	0.0066 (18)	−0.020 (2)	−0.0088 (18)
N21	0.0509 (17)	0.0262 (13)	0.0405 (16)	−0.0023 (11)	−0.0030 (13)	−0.0075 (11)
C22	0.059 (2)	0.0296 (16)	0.046 (2)	−0.0009 (15)	0.0001 (16)	−0.0057 (14)
O22	0.116 (3)	0.0435 (16)	0.0472 (17)	−0.0018 (17)	−0.0089 (17)	−0.0079 (13)
C23	0.076 (3)	0.0267 (17)	0.059 (2)	−0.0025 (17)	0.000 (2)	−0.0010 (16)
C30	0.076 (3)	0.0427 (19)	0.0384 (19)	−0.0026 (18)	0.0052 (18)	−0.0136 (15)
C31	0.073 (3)	0.077 (3)	0.074 (3)	0.010 (3)	0.010 (3)	−0.018 (3)
C32	0.124 (5)	0.109 (5)	0.053 (3)	−0.026 (4)	0.006 (3)	−0.042 (3)
O51	0.0637 (17)	0.0370 (13)	0.0571 (17)	0.0050 (12)	−0.0174 (13)	−0.0090 (12)
C52	0.080 (3)	0.042 (2)	0.072 (3)	0.009 (2)	−0.016 (2)	−0.012 (2)
O52	0.190 (5)	0.053 (2)	0.140 (4)	0.045 (3)	−0.102 (4)	−0.030 (2)
C53	0.105 (4)	0.051 (3)	0.096 (4)	−0.009 (3)	−0.027 (3)	−0.020 (3)
N11	0.0390 (15)	0.0443 (16)	0.0367 (16)	−0.0083 (12)	0.0010 (12)	−0.0116 (13)
C12	0.0315 (16)	0.0342 (16)	0.0421 (17)	−0.0051 (12)	0.0006 (13)	−0.0093 (13)
N13	0.0404 (14)	0.0310 (13)	0.0368 (14)	−0.0057 (11)	−0.0001 (11)	−0.0121 (11)

C14	0.0284 (14)	0.0332 (15)	0.0356 (16)	−0.0027 (11)	0.0016 (12)	−0.0124 (12)
C15	0.0287 (15)	0.0352 (16)	0.0442 (18)	−0.0055 (12)	0.0005 (13)	−0.0157 (13)
C16	0.0292 (15)	0.0450 (19)	0.0477 (19)	−0.0066 (13)	0.0014 (13)	−0.0206 (15)
O16	0.0605 (17)	0.0562 (16)	0.0483 (15)	−0.0084 (13)	−0.0015 (13)	−0.0286 (13)
N17	0.0382 (15)	0.0339 (14)	0.0525 (18)	−0.0047 (11)	−0.0045 (13)	−0.0169 (13)
C18	0.0431 (18)	0.0304 (16)	0.049 (2)	−0.0032 (13)	−0.0052 (15)	−0.0090 (14)
N19	0.0372 (14)	0.0308 (13)	0.0381 (14)	−0.0028 (10)	−0.0033 (11)	−0.0103 (11)
C11'	0.0388 (17)	0.0360 (16)	0.0355 (16)	−0.0008 (13)	0.0008 (13)	−0.0099 (13)
C12'	0.0409 (17)	0.0377 (16)	0.0393 (17)	−0.0041 (13)	0.0014 (13)	−0.0188 (14)
O11	0.0519 (15)	0.0558 (16)	0.0373 (13)	−0.0144 (12)	−0.0004 (11)	−0.0048 (11)
O12	0.0701 (18)	0.0383 (13)	0.0432 (14)	0.0071 (12)	−0.0075 (12)	−0.0191 (11)
O13	0.106 (3)	0.0621 (19)	0.0417 (15)	0.0282 (18)	−0.0193 (16)	−0.0249 (14)
C13'	0.049 (2)	0.050 (2)	0.0450 (19)	0.0072 (15)	−0.0116 (16)	−0.0230 (17)
C14'	0.053 (2)	0.049 (2)	0.0337 (17)	0.0011 (16)	−0.0068 (15)	−0.0089 (15)
C15'	0.067 (3)	0.048 (2)	0.054 (2)	0.0102 (19)	−0.016 (2)	−0.0175 (18)
N121	0.0481 (17)	0.0351 (15)	0.0480 (17)	−0.0066 (12)	−0.0029 (13)	−0.0065 (13)
C122	0.053 (2)	0.047 (2)	0.049 (2)	−0.0040 (17)	−0.0011 (17)	−0.0008 (18)
O122	0.096 (3)	0.063 (2)	0.0476 (18)	−0.0009 (18)	−0.0051 (16)	−0.0019 (15)
C123	0.075 (3)	0.048 (2)	0.074 (3)	−0.001 (2)	−0.008 (2)	0.005 (2)
C130	0.072 (3)	0.0396 (18)	0.0404 (19)	0.0042 (17)	−0.0028 (17)	−0.0183 (15)
C131	0.139 (6)	0.091 (4)	0.072 (4)	−0.048 (4)	−0.008 (4)	−0.039 (3)
C132	0.088 (4)	0.105 (5)	0.055 (3)	0.016 (3)	0.017 (3)	−0.011 (3)
O151	0.0605 (19)	0.0502 (18)	0.107 (3)	0.0030 (14)	−0.0225 (19)	−0.0259 (18)
C152	0.075 (3)	0.060 (3)	0.072 (3)	0.006 (2)	−0.017 (3)	−0.016 (2)
O152	0.134 (5)	0.103 (4)	0.130 (5)	−0.037 (4)	−0.036 (4)	0.043 (3)
C153	0.086 (4)	0.105 (5)	0.119 (6)	0.038 (4)	−0.052 (4)	−0.048 (4)
O1W	0.092 (2)	0.0366 (14)	0.074 (2)	−0.0037 (14)	−0.0163 (17)	−0.0247 (14)
O2W	0.071 (2)	0.0555 (18)	0.085 (2)	−0.0057 (15)	0.0044 (17)	−0.0409 (17)

Geometric parameters (Å, °)

N1—C2	1.373 (4)	N11—H11	0.89 (5)
N1—C6	1.410 (4)	C12—N13	1.306 (5)
N1—H1	0.77 (6)	C12—N121	1.396 (4)
C2—N3	1.303 (4)	N13—C14	1.357 (4)
C2—N21	1.383 (4)	C14—N19	1.366 (4)
N3—C4	1.356 (4)	C14—C15	1.387 (4)
C4—N9	1.374 (4)	C15—N17	1.387 (5)
C4—C5	1.383 (4)	C15—C16	1.437 (5)
C5—N7	1.393 (4)	C16—O16	1.224 (4)
C5—C6	1.431 (5)	N17—C18	1.299 (5)
C6—O6	1.227 (4)	C18—N19	1.383 (4)
N7—C8	1.310 (5)	C18—H18	0.930
C8—N9	1.373 (4)	N19—C11'	1.483 (4)
C8—H8	0.930	C11'—O11	1.408 (4)
N9—C1'	1.455 (4)	C11'—C12'	1.536 (5)
C1'—O1	1.404 (4)	C11'—H11'	0.980
C1'—C2'	1.508 (5)	C12'—O12	1.420 (4)
C1'—H1'	0.980	C12'—C13'	1.536 (5)

C2'—O2	1.427 (4)	C12'—H12'	0.980
C2'—C3'	1.526 (5)	O11—C14'	1.438 (5)
C2'—H2'	0.980	O12—C130	1.445 (5)
C3'—O3	1.410 (5)	O13—C130	1.423 (5)
C3'—C4'	1.516 (6)	O13—C13'	1.432 (5)
C3'—H3'	0.980	C13'—C14'	1.498 (6)
O1—C4'	1.440 (5)	C13'—H13'	0.980
O2—C30	1.429 (5)	C14'—C15'	1.503 (6)
O3—C30	1.441 (5)	C14'—H14'	0.980
C4'—C5'	1.502 (5)	C15'—O151	1.413 (5)
C4'—H4'	0.980	C15'—H15A	0.970
C5'—O51	1.445 (5)	C15'—H15B	0.970
C5'—H5'1	0.970	N121—C122	1.375 (5)
C5'—H5'2	0.970	N121—H121	0.95 (5)
N21—C22	1.360 (5)	C122—O122	1.221 (6)
N21—H21	0.89 (4)	C122—C123	1.503 (7)
C22—O22	1.220 (5)	C123—H12A	0.960
C22—C23	1.518 (5)	C123—H12B	0.960
C23—H23A	0.960	C123—H12C	0.960
C23—H23B	0.960	C130—C131	1.483 (7)
C23—H23C	0.960	C130—C132	1.492 (7)
C30—C31	1.473 (7)	C131—H13A	0.960
C30—C32	1.504 (7)	C131—H13B	0.960
C31—H31A	0.960	C131—H13C	0.960
C31—H31B	0.960	C132—H13D	0.960
C31—H31C	0.960	C132—H13E	0.960
C32—H32A	0.960	C132—H13F	0.960
C32—H32B	0.960	O151—C152	1.319 (6)
C32—H32C	0.960	C152—O152	1.156 (8)
O51—C52	1.334 (5)	C152—C153	1.487 (8)
C52—O52	1.188 (6)	C153—H15C	0.960
C52—C53	1.478 (8)	C153—H15D	0.960
C53—H53A	0.960	C153—H15E	0.960
C53—H53B	0.960	O1W—H1WA	0.8719
C53—H53C	0.960	O1W—H1WB	0.8614
N11—C12	1.359 (5)	O2W—H2WA	0.9113
N11—C16	1.415 (5)	O2W—H2WB	0.8654
C2—N1—C6	125.4 (3)	C12—N11—H11	117 (3)
C2—N1—H1	113 (4)	C16—N11—H11	118 (3)
C6—N1—H1	122 (4)	N13—C12—N11	125.1 (3)
N3—C2—N1	124.9 (3)	N13—C12—N121	115.9 (3)
N3—C2—N21	117.0 (3)	N11—C12—N121	118.9 (3)
N1—C2—N21	118.1 (3)	C12—N13—C14	111.8 (3)
C2—N3—C4	111.5 (3)	N13—C14—N19	125.0 (3)
N3—C4—N9	125.0 (3)	N13—C14—C15	128.6 (3)
N3—C4—C5	129.0 (3)	N19—C14—C15	106.4 (3)
N9—C4—C5	106.0 (3)	N17—C15—C14	110.0 (3)
C4—C5—N7	110.0 (3)	N17—C15—C16	131.2 (3)
C4—C5—C6	119.0 (3)	C14—C15—C16	118.7 (3)

N7—C5—C6	131.0 (3)	O16—C16—N11	120.3 (3)
O6—C6—N1	119.7 (3)	O16—C16—C15	129.4 (3)
O6—C6—C5	130.1 (3)	N11—C16—C15	110.3 (3)
N1—C6—C5	110.2 (3)	C18—N17—C15	104.4 (3)
C8—N7—C5	104.6 (3)	N17—C18—N19	113.9 (3)
N7—C8—N9	113.1 (3)	N17—C18—H18	123.1
N7—C8—H8	123.5	N19—C18—H18	123.1
N9—C8—H8	123.5	C14—N19—C18	105.3 (3)
C8—N9—C4	106.2 (3)	C14—N19—C11'	125.4 (3)
C8—N9—C1'	128.1 (3)	C18—N19—C11'	128.3 (3)
C4—N9—C1'	125.6 (3)	O11—C11'—N19	108.8 (3)
O1—C1'—N9	107.8 (3)	O11—C11'—C12'	108.1 (3)
O1—C1'—C2'	107.0 (3)	N19—C11'—C12'	112.5 (3)
N9—C1'—C2'	112.3 (3)	O11—C11'—H11'	109.1
O1—C1'—H1'	109.9	N19—C11'—H11'	109.1
N9—C1'—H1'	109.9	C12'—C11'—H11'	109.1
C2'—C1'—H1'	109.9	O12—C12'—C13'	105.3 (3)
O2—C2'—C1'	109.5 (3)	O12—C12'—C11'	113.5 (3)
O2—C2'—C3'	101.1 (3)	C13'—C12'—C11'	103.0 (3)
C1'—C2'—C3'	105.4 (3)	O12—C12'—H12'	111.5
O2—C2'—H2'	113.3	C13'—C12'—H12'	111.5
C1'—C2'—H2'	113.3	C11'—C12'—H12'	111.5
C3'—C2'—H2'	113.3	C11'—O11—C14'	109.9 (3)
O3—C3'—C4'	112.9 (3)	C12'—O12—C130	109.2 (3)
O3—C3'—C2'	105.1 (3)	C130—O13—C13'	108.6 (3)
C4'—C3'—C2'	102.7 (3)	O13—C13'—C14'	109.4 (4)
O3—C3'—H3'	111.9	O13—C13'—C12'	103.2 (3)
C4'—C3'—H3'	111.9	C14'—C13'—C12'	105.6 (3)
C2'—C3'—H3'	111.9	O13—C13'—H13'	112.7
C1'—O1—C4'	111.5 (3)	C14'—C13'—H13'	112.7
C2'—O2—C30	107.3 (3)	C12'—C13'—H13'	112.7
C3'—O3—C30	108.8 (3)	O11—C14'—C13'	104.6 (3)
O1—C4'—C5'	108.8 (3)	O11—C14'—C15'	108.5 (3)
O1—C4'—C3'	105.9 (3)	C13'—C14'—C15'	113.5 (4)
C5'—C4'—C3'	117.2 (3)	O11—C14'—H14'	110.0
O1—C4'—H4'	108.2	C13'—C14'—H14'	110.0
C5'—C4'—H4'	108.2	C15'—C14'—H14'	110.0
C3'—C4'—H4'	108.2	O151—C15'—C14'	110.5 (3)
O51—C5'—C4'	107.6 (3)	O151—C15'—H15A	109.6
O51—C5'—H5'1	110.2	C14'—C15'—H15A	109.6
C4'—C5'—H5'1	110.2	O151—C15'—H15B	109.6
O51—C5'—H5'2	110.2	C14'—C15'—H15B	109.6
C4'—C5'—H5'2	110.2	H15A—C15'—H15B	108.1
H5'1—C5'—H5'2	108.5	C122—N121—C12	127.9 (4)
C22—N21—C2	126.9 (3)	C122—N121—H121	120 (3)
C22—N21—H21	121 (2)	C12—N121—H121	112 (3)
C2—N21—H21	112 (2)	O122—C122—N121	121.9 (4)
O22—C22—N21	123.7 (3)	O122—C122—C123	124.2 (4)
O22—C22—C23	122.3 (4)	N121—C122—C123	113.9 (4)

N21—C22—C23	114.0 (3)	C122—C123—H12A	109.5
C22—C23—H23A	109.5	C122—C123—H12B	109.5
C22—C23—H23B	109.5	H12A—C123—H12B	109.5
H23A—C23—H23B	109.5	C122—C123—H12C	109.5
C22—C23—H23C	109.5	H12A—C123—H12C	109.5
H23A—C23—H23C	109.5	H12B—C123—H12C	109.5
H23B—C23—H23C	109.5	O13—C130—O12	106.8 (3)
O2—C30—O3	105.4 (3)	O13—C130—C131	113.2 (5)
O2—C30—C31	110.0 (4)	O12—C130—C131	109.0 (4)
O3—C30—C31	108.3 (4)	O13—C130—C132	106.4 (4)
O2—C30—C32	107.9 (4)	O12—C130—C132	108.9 (4)
O3—C30—C32	110.3 (4)	C131—C130—C132	112.2 (5)
C31—C30—C32	114.6 (5)	C130—C131—H13A	109.5
C30—C31—H31A	109.5	C130—C131—H13B	109.5
C30—C31—H31B	109.5	H13A—C131—H13B	109.5
H31A—C31—H31B	109.5	C130—C131—H13C	109.5
C30—C31—H31C	109.5	H13A—C131—H13C	109.5
H31A—C31—H31C	109.5	H13B—C131—H13C	109.5
H31B—C31—H31C	109.5	C130—C132—H13D	109.5
C30—C32—H32A	109.5	C130—C132—H13E	109.5
C30—C32—H32B	109.5	H13D—C132—H13E	109.5
H32A—C32—H32B	109.5	C130—C132—H13F	109.5
C30—C32—H32C	109.5	H13D—C132—H13F	109.5
H32A—C32—H32C	109.5	H13E—C132—H13F	109.5
H32B—C32—H32C	109.5	C152—O151—C15'	117.6 (4)
C52—O51—C5'	116.9 (3)	O152—C152—O151	122.2 (5)
O52—C52—O51	122.1 (5)	O152—C152—C153	126.6 (6)
O52—C52—C53	125.7 (5)	O151—C152—C153	111.1 (6)
O51—C52—C53	112.2 (4)	C152—C153—H15C	109.5
C52—C53—H53A	109.5	C152—C153—H15D	109.5
C52—C53—H53B	109.5	H15C—C153—H15D	109.5
H53A—C53—H53B	109.5	C152—C153—H15E	109.5
C52—C53—H53C	109.5	H15C—C153—H15E	109.5
H53A—C53—H53C	109.5	H15D—C153—H15E	109.5
H53B—C53—H53C	109.5	H1WA—O1W—H1WB	109.3
C12—N11—C16	125.4 (3)	H2WA—O2W—H2WB	109.5
C6—N1—C2—N3	−0.4 (5)	C16—N11—C12—N13	−2.4 (5)
C6—N1—C2—N21	179.7 (3)	C16—N11—C12—N121	177.5 (3)
N1—C2—N3—C4	0.8 (4)	N11—C12—N13—C14	1.8 (5)
N21—C2—N3—C4	−179.2 (3)	N121—C12—N13—C14	−178.1 (3)
C2—N3—C4—N9	179.0 (3)	C12—N13—C14—N19	177.5 (3)
C2—N3—C4—C5	−0.9 (5)	C12—N13—C14—C15	−0.7 (5)
N3—C4—C5—N7	−179.9 (3)	N13—C14—C15—N17	177.3 (3)
N9—C4—C5—N7	0.2 (3)	N19—C14—C15—N17	−1.2 (4)
N3—C4—C5—C6	0.5 (5)	N13—C14—C15—C16	0.2 (5)
N9—C4—C5—C6	−179.5 (3)	N19—C14—C15—C16	−178.3 (3)
C2—N1—C6—O6	−179.9 (3)	C12—N11—C16—O16	−177.3 (3)
C2—N1—C6—C5	−0.1 (4)	C12—N11—C16—C15	1.5 (4)
C4—C5—C6—O6	179.8 (3)	N17—C15—C16—O16	1.7 (6)

N7—C5—C6—O6	0.2 (6)	C14—C15—C16—O16	178.1 (3)
C4—C5—C6—N1	0.1 (4)	N17—C15—C16—N11	−176.9 (3)
N7—C5—C6—N1	−179.5 (3)	C14—C15—C16—N11	−0.5 (4)
C4—C5—N7—C8	−0.3 (4)	C14—C15—N17—C18	0.0 (4)
C6—C5—N7—C8	179.3 (3)	C16—C15—N17—C18	176.7 (3)
C5—N7—C8—N9	0.4 (4)	C15—N17—C18—N19	1.2 (4)
N7—C8—N9—C4	−0.3 (4)	N13—C14—N19—C18	−176.8 (3)
N7—C8—N9—C1'	−178.9 (3)	C15—C14—N19—C18	1.8 (3)
N3—C4—N9—C8	−179.9 (3)	N13—C14—N19—C11'	−7.1 (5)
C5—C4—N9—C8	0.0 (3)	C15—C14—N19—C11'	171.5 (3)
N3—C4—N9—C1'	−1.3 (5)	N17—C18—N19—C14	−2.0 (4)
C5—C4—N9—C1'	178.7 (3)	N17—C18—N19—C11'	−171.3 (3)
C8—N9—C1'—O1	38.3 (5)	C14—N19—C11'—O11	−178.9 (3)
C4—N9—C1'—O1	−140.0 (3)	C18—N19—C11'—O11	−11.6 (4)
C8—N9—C1'—C2'	−79.4 (4)	C14—N19—C11'—C12'	61.3 (4)
C4—N9—C1'—C2'	102.3 (4)	C18—N19—C11'—C12'	−131.4 (3)
O1—C1'—C2'—O2	92.1 (3)	O11—C11'—C12'—O12	114.1 (3)
N9—C1'—C2'—O2	−149.7 (3)	N19—C11'—C12'—O12	−125.7 (3)
O1—C1'—C2'—C3'	−15.9 (4)	O11—C11'—C12'—C13'	0.8 (3)
N9—C1'—C2'—C3'	102.2 (3)	N19—C11'—C12'—C13'	121.0 (3)
O2—C2'—C3'—O3	29.8 (4)	N19—C11'—O11—C14'	−104.6 (3)
C1'—C2'—C3'—O3	143.9 (3)	C12'—C11'—O11—C14'	17.9 (4)
O2—C2'—C3'—C4'	−88.5 (3)	C13'—C12'—O12—C130	10.4 (4)
C1'—C2'—C3'—C4'	25.6 (4)	C11'—C12'—O12—C130	−101.5 (4)
N9—C1'—O1—C4'	−122.1 (3)	C130—O13—C13'—C14'	138.7 (4)
C2'—C1'—O1—C4'	−1.1 (4)	C130—O13—C13'—C12'	26.6 (5)
C1'—C2'—O2—C30	−146.2 (3)	O12—C12'—C13'—O13	−22.4 (4)
C3'—C2'—O2—C30	−35.3 (4)	C11'—C12'—C13'—O13	96.8 (3)
C4'—C3'—O3—C30	97.3 (4)	O12—C12'—C13'—C14'	−137.2 (3)
C2'—C3'—O3—C30	−13.9 (4)	C11'—C12'—C13'—C14'	−18.0 (4)
C1'—O1—C4'—C5'	144.7 (3)	C11'—O11—C14'—C13'	−29.4 (4)
C1'—O1—C4'—C3'	17.8 (4)	C11'—O11—C14'—C15'	92.1 (4)
O3—C3'—C4'—O1	−139.0 (3)	O13—C13'—C14'—O11	−81.7 (4)
C2'—C3'—C4'—O1	−26.4 (4)	C12'—C13'—C14'—O11	28.8 (4)
O3—C3'—C4'—C5'	99.4 (4)	O13—C13'—C14'—C15'	160.1 (3)
C2'—C3'—C4'—C5'	−147.9 (3)	C12'—C13'—C14'—C15'	−89.3 (4)
O1—C4'—C5'—O51	−69.8 (4)	O11—C14'—C15'—O151	168.8 (4)
C3'—C4'—C5'—O51	50.2 (5)	C13'—C14'—C15'—O151	−75.3 (4)
N3—C2—N21—C22	−179.0 (3)	N13—C12—N121—C122	175.0 (4)
N1—C2—N21—C22	0.9 (5)	N11—C12—N121—C122	−4.9 (5)
C2—N21—C22—O22	3.1 (7)	C12—N121—C122—O122	0.1 (7)
C2—N21—C22—C23	−176.7 (4)	C12—N121—C122—C123	−178.5 (4)
C2'—O2—C30—O3	28.0 (4)	C13'—O13—C130—O12	−21.0 (5)
C2'—O2—C30—C31	−88.6 (4)	C13'—O13—C130—C131	98.9 (5)
C2'—O2—C30—C32	145.8 (4)	C13'—O13—C130—C132	−137.3 (4)
C3'—O3—C30—O2	−7.7 (5)	C12'—O12—C130—O13	5.8 (5)
C3'—O3—C30—C31	110.0 (4)	C12'—O12—C130—C131	−116.9 (5)
C3'—O3—C30—C32	−123.8 (4)	C12'—O12—C130—C132	120.4 (4)
C4'—C5'—O51—C52	−170.8 (4)	C14'—C15'—O151—C152	−105.0 (5)

C5'—O51—C52—O52	0.0 (9)	C15'—O151—C152—O152	2.8 (9)
C5'—O51—C52—C53	−179.7 (5)	C15'—O151—C152—C153	−174.4 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O22	0.77 (6)	2.00 (6)	2.649 (4)	142 (5)
N11—H11···O122	0.89 (5)	2.01 (5)	2.690 (5)	133 (4)
N21—H21···O1W^{i}	0.89 (4)	1.88 (4)	2.757 (4)	168 (4)
N121—H121···O2W^{ii}	0.95 (5)	1.98 (5)	2.915 (5)	169 (4)
O2W—H2WA···N17	0.91	2.00	2.885 (4)	162
O1W—H1WA···N7	0.87	1.91	2.775 (4)	173
O2W—H2WB···O1W^{iii}	0.87	2.15	3.011 (5)	170

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

Fig. 1

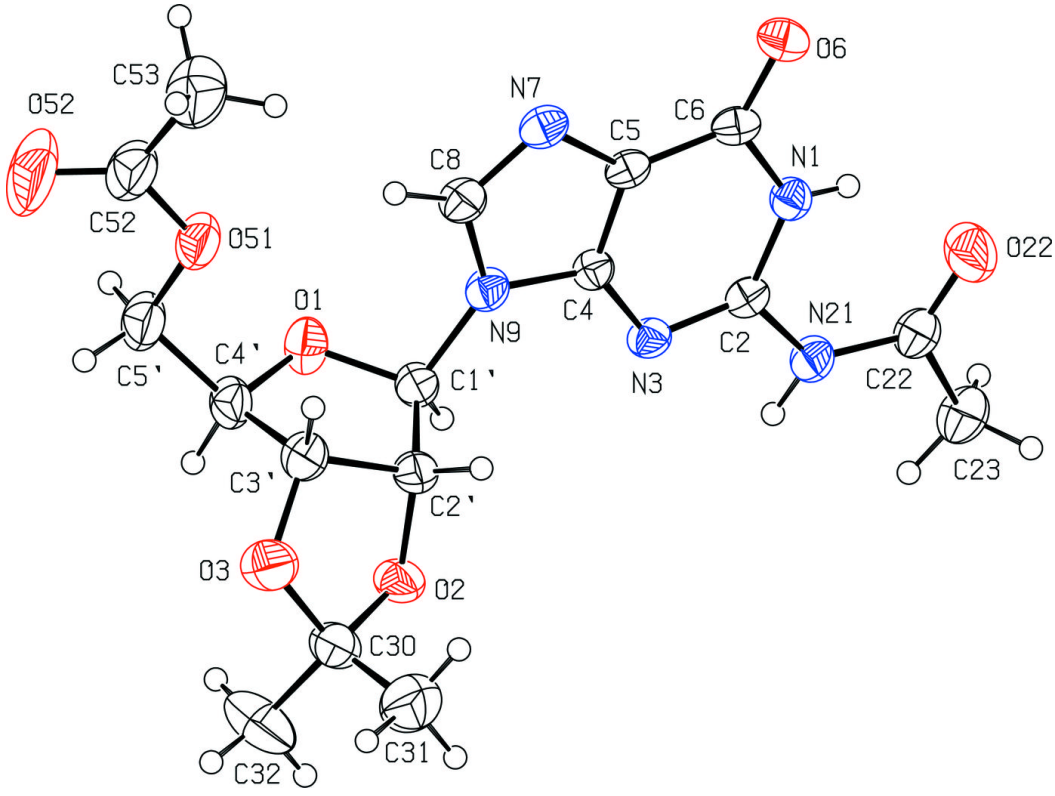

C53
O52
C52
O51
C5'
C4'
O1
C1'
C3'
C2'
O3
O2
C30
C32
C31
N9
C8
N7
C5
C6
O6
N1
C4
N3
C2
N21
C22
O22
C23

Fig. 2

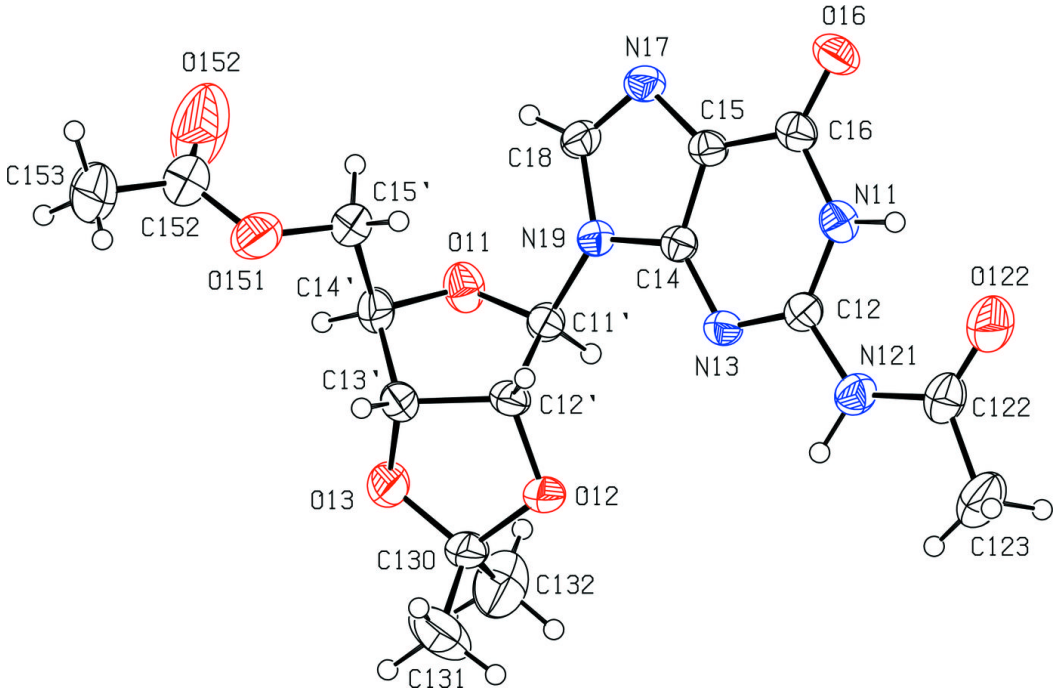

O16
N17
O152
C15
C16
C153
C18
C15'
N11
C152
O11
N19
C14
O122
O151
C14'
C12
C11'
N13
N121
C13'
C12'
C122
O13
O12
C123
C130
C132
C131

Fig. 3