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5-Phenyluridine trihydrate

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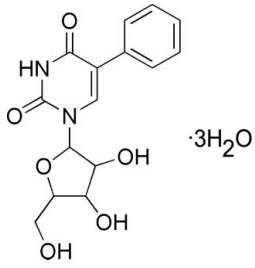
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; H-atom completeness 73%; disorder in solvent or counterion; R factor = 0.053; wR factor = 0.185; data-to-parameter ratio = 11.3.

The title compound (systematic name: 2,4-dihydroxy-5-phenyl-1-β-D-ribofuranosylpyrimidine trihydrate), crystallized as the trihydrate, $C_{15}H_{16}N_2O_6\cdot3H_2O$, stabilized by hydrogen bonds to the uracil O atoms. Two statistically disordered water solvent molecules occupy channels along the a axis; the site occupancy factors are *ca* 0.6 and 0.4. The heterocyclic base is almost planar and is oriented *anti* with respect to the puckered sugar moiety. The sugar ring adopts a conformation intermediate between twist and envelope.

Related literature

For related literature, see: Ali *et al.* (2006); Aucagne *et al.* (2006); Cremer & Pople (1975); Flack (1983); Flack & Bernardinelli (2000); Flynn *et al.* (1991); Rai *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{16}N_2O_6\cdot3H_2O$
M_r = 374.35
Orthorhombic, $P2_12_12_1$
a = 7.3627 (1) Å
b = 14.0874 (3) Å
c = 16.7287 (3) Å
V = 1735.12 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 (2) K
0.45 × 0.24 × 0.14 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
5050 measured reflections
2879 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.185
S = 1.16
2879 reflections
255 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3′^{i}	0.86	2.02	2.842 (3)	159
O2′—H2O′···O2^{ii}	0.82	2.00	2.740 (3)	151
O3′—H3O′···O3W^{iii}	0.82	1.83	2.600 (9)	157
O3′—H3O′···O3W'^{iii}	0.82	1.88	2.691 (9)	169
O5′—H5O′···O2′^{iv}	0.82	1.92	2.735 (3)	171

Symmetry codes: (i) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, -y+1, z+\frac{1}{2}$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RT2004).

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supplementary materials

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5-Phenyluridine trihydrate

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Comment

Research has been focused towards finding biologically active analogues of uridine, a naturally occurring compound, and modification of the uracil ring concentrates on position 5. Examples of the latest investigations for the development of new drugs include *e.g.* the synthesis of ethynyl uridine derivatives as antiviral drugs against Flaviviridae (Aucagne *et al.*, 2006), especially HCV, studies of other alkynyl-uridines as potent inhibitors of Mycobacteria (Rai *et al.*, 2005), and *e.g.* uridine and estradiol conjugates exhibiting binding affinity and cytotoxicity against cell lines with and without an estrogen receptor (Ali, H. *et al.*, 2006). Modern synthetic methods include coupling reactions with catalysis by organometallic compounds, which enables the introduction of diverse substituents of an aliphatic or aromatic nature. Although the synthesis and biological activity of uridine derivatives has been studied intensively, their structural parameters from crystallographic measurements, important for behavior in biological systems, have rarely been discussed and published. In this paper we describe the structural properties of 5-phenyluridine prepared by the Suzuki coupling from 5-iodouridine and phenylboronic acid.

A selection of geometric parameters is given in Table 1. The heterocyclic base moiety is almost planar, with a maximum deviation of 0.019 (3) Å for the C1 atom. The N-glycosidic torsion angle χ (C1–N1–C1'–O4') is −169.8 (2)° which corresponds to an *anti* orientation of the base moiety. The sugar ring, C1'–C2'–C3'–C4'–O4', adopts a mixed twisted- envelope $^{3}T_{2}/^{3}E$ conformation (C3'-*exo* / C2'-*endo*) with puckering parameters q_2 = 0.384 (3) Å and φ_2 = 64.2 (4)° (Cremer & Pople, 1975). The conformation of the side chain, as defined by the torsion angle O5'–C5'–C4'–C3' of 53.5 (3)°, is +*sc*. The phenyl and uracil rings are not co-planar (Fig.1), with a dihedral angle between the mean planes of 38.02 (9)°. The crystal packing is determined by a network of hydrogen bonds (Table 2) with π-π interactions (3.455 Å) observed between the phenyl and uracil moieties. This packing creates channels along the *a* axis which hosts the solvent molecules (Fig. 2).

Experimental

5-phenyluridine was prepared by the Suzuki coupling reaction of 5-iodouridine (0.277 g, 0.75 mmol) and phenylboronic acid (0.081 g, 0.90 mmol) (Flynn *et al.* 1991), yield 0.203 g (84%). Analytical data are identical with that published. The final product was obtained from slow evaporation of an aqueous solution (10 mg/ml) at room temperature. MS: m/*z* 321.

Refinement

The aromatic, methylene, methine, amine and hydroxyl H atoms were placed in geometrically idealized positions (C—H = 0.93–0.98, N—H = 0.86 and O—H = 0.82 Å) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C,*N*,*O*). Water molecules O1W and O3W refined with large thermal vibrations and were subsequently refined disordered over two sites as O1W/O1W' and O3W/O3W' respectively. Refinement was kept stable with the use of anisotropic restraints and free variables were incorporated to refine occupation parameters to one. Possible hydogen coordinates from the Fourier difference map could not be refined satisfactory. Refinement of the Flack parameter (Flack, 1983) led to an inconclusive value (Flack & Bernardinelli, 2000) of −10 (10). This is generally the case with light atom Mo *K*α data where f" is nearly

zero. The Friedel equivalents were therefore merged before final refinement with a MERG 4 command. The conformation of the title compound was assigned from the absolute configuration of the starting material.

Figures

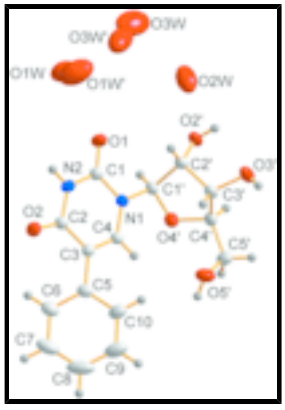

Fig. 1. The structure of (1) showing the displacement ellipsoids parameters at 50% probability.

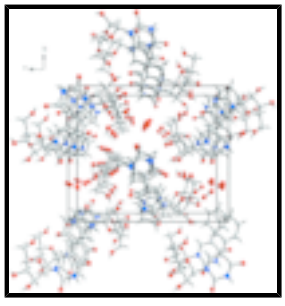

Fig. 2. The crystal packing of (1) viewed down the crystallographic *a* axis

2,4-dihydroxy-5-phenyl-1-β-*D*-ribofuranosylpyrimidine trihydrate

Crystal data

$C_{15}H_{16}N_2O_6 \cdot 3H_2O$	F_{000} = 792
M_r = 374.35	D_x = 1.433 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2838 reflections
a = 7.36270 (10) Å	θ = 3.9–30°
b = 14.0874 (3) Å	μ = 0.12 mm^{-1}
c = 16.7287 (3) Å	T = 295 (2) K
V = 1735.12 (5) Å^3	Prismatic, colourless
Z = 4	0.45 × 0.24 × 0.14 mm

Data collection

Nonius KappaCCD diffractometer	2338 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 295(2) K	θ_{max} = 30.0°

φ and ω scans	θ_{min} = 1.9º
Absorption correction: none	h = −10→10
5050 measured reflections	k = −19→19
2879 independent reflections	l = −23→23

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1267P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$\Delta\rho_{max} = 0.63$ e Å^{-3}
$wR(F^2) = 0.185$	$\Delta\rho_{min} = -0.63$ e Å^{-3}
S = 1.16	Extinction correction: none
2879 reflections	
255 parameters	
12 restraints	
H-atom parameters constrained	

Special details

Experimental. The diffraction data were collected at room temperature using a Nonius Kappa CCD diffractometer with graphite-monochromated Mo Kα (λ = 0.7107 Å) using an exposure time of 40 s/frame. A total of 204 frames were collected with a frame width of 2.0° covering up to θ = 30.04° with 99.6% completeness accomplished.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.8933 (4)	0.55845 (14)	0.57391 (13)	0.0405 (5)	
O2	0.7725 (3)	0.33876 (14)	0.38352 (11)	0.0349 (5)	
N1	0.9232 (3)	0.40257 (16)	0.60850 (12)	0.0262 (4)	
N2	0.8299 (3)	0.44486 (15)	0.48118 (14)	0.0296 (5)	
H2	0.7984	0.4885	0.448	0.036*	
C1	0.8832 (4)	0.47460 (19)	0.55542 (16)	0.0283 (5)	
C2	0.8209 (4)	0.35266 (17)	0.45353 (15)	0.0254 (5)	
C3	0.8698 (4)	0.28058 (17)	0.51060 (15)	0.0246 (5)	
C4	0.9212 (4)	0.30928 (18)	0.58495 (15)	0.0250 (5)	
H4	0.9567	0.2633	0.6216	0.03*	
C5	0.8662 (4)	0.17852 (19)	0.48985 (16)	0.0286 (5)	
C6	0.9221 (4)	0.1455 (2)	0.41495 (19)	0.0365 (6)	
H6	0.9593	0.1886	0.3762	0.044*	
C7	0.9225 (5)	0.0498 (3)	0.3980 (2)	0.0496 (9)	
H7	0.9604	0.0289	0.348	0.059*	
C8	0.8669 (5)	−0.0158 (2)	0.4549 (3)	0.0585 (11)	

H8	0.8687	−0.0804	0.4433	0.07*	
C9	0.8084 (6)	0.0157 (2)	0.5297 (3)	0.0521 (9)	
H9	0.7698	−0.0275	0.5681	0.063*	
C10	0.8083 (5)	0.1124 (2)	0.5461 (2)	0.0392 (7)	
H10	0.7687	0.1334	0.5958	0.047*	
C1'	0.9934 (4)	0.43348 (18)	0.68847 (14)	0.0255 (5)	
H1'	1.0928	0.4789	0.6812	0.031*	
C2'	0.8448 (4)	0.47799 (17)	0.73959 (15)	0.0264 (5)	
H2'	0.75	0.5086	0.7076	0.032*	
O2'	0.9353 (3)	0.54254 (13)	0.79151 (12)	0.0327 (5)	
H2O'	0.8655	0.5595	0.8269	0.039*	
C3'	0.7751 (4)	0.39195 (18)	0.78564 (15)	0.0285 (5)	
H3'	0.6943	0.3544	0.7515	0.034*	
O3'	0.6828 (3)	0.41854 (14)	0.85632 (14)	0.0433 (6)	
H3O'	0.6012	0.3804	0.8654	0.052*	
C4'	0.9494 (4)	0.33734 (19)	0.80117 (15)	0.0307 (6)	
H4'	1.0118	0.3665	0.8467	0.037*	
O4'	1.0571 (3)	0.35341 (14)	0.73006 (11)	0.0318 (4)	
C5'	0.9330 (5)	0.2329 (2)	0.81655 (18)	0.0395 (7)	
H51'	1.0535	0.2055	0.8211	0.047*	
H52'	0.8706	0.2229	0.8669	0.047*	
O5'	0.8359 (3)	0.18558 (16)	0.75411 (14)	0.0437 (6)	
H5O'	0.8947	0.1397	0.7387	0.052*	
O1W	0.831 (2)	0.7382 (6)	0.5078 (5)	0.083 (4)	0.63 (3)
O1W'	0.715 (5)	0.7221 (11)	0.5193 (16)	0.114 (7)	0.37 (3)
O2W	0.5372 (5)	0.6628 (3)	0.7329 (2)	0.0838 (12)	
O3W	0.6219 (14)	0.8252 (13)	0.6464 (15)	0.107 (6)	0.43 (3)
O3W'	0.549 (3)	0.7790 (12)	0.6033 (9)	0.118 (7)	0.57 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0665 (14)	0.0226 (9)	0.0324 (10)	−0.0004 (9)	−0.0019 (11)	−0.0011 (8)
O2	0.0495 (11)	0.0311 (9)	0.0242 (9)	0.0031 (9)	−0.0093 (9)	0.0009 (7)
N1	0.0367 (11)	0.0226 (9)	0.0192 (9)	0.0029 (9)	−0.0005 (9)	−0.0021 (7)
N2	0.0426 (12)	0.0211 (9)	0.0251 (10)	0.0032 (9)	−0.0038 (10)	0.0027 (8)
C1	0.0362 (13)	0.0233 (11)	0.0253 (12)	0.0017 (10)	0.0000 (10)	0.0018 (9)
C2	0.0302 (12)	0.0228 (11)	0.0232 (11)	−0.0002 (10)	−0.0016 (9)	−0.0008 (9)
C3	0.0285 (11)	0.0216 (10)	0.0237 (11)	0.0007 (9)	0.0005 (10)	0.0012 (9)
C4	0.0312 (12)	0.0214 (10)	0.0223 (11)	0.0023 (10)	−0.0004 (10)	−0.0005 (9)
C5	0.0302 (12)	0.0247 (12)	0.0310 (13)	0.0036 (10)	−0.0073 (10)	−0.0027 (10)
C6	0.0360 (14)	0.0333 (14)	0.0402 (15)	0.0040 (12)	−0.0022 (13)	−0.0079 (12)
C7	0.0438 (17)	0.0410 (17)	0.064 (2)	0.0118 (15)	−0.0104 (17)	−0.0229 (16)
C8	0.057 (2)	0.0272 (14)	0.091 (3)	0.0060 (15)	−0.029 (2)	−0.0150 (17)
C9	0.065 (2)	0.0270 (13)	0.064 (2)	−0.0065 (15)	−0.019 (2)	0.0062 (15)
C10	0.0516 (17)	0.0263 (13)	0.0398 (15)	−0.0017 (13)	−0.0094 (14)	0.0039 (11)
C1'	0.0319 (11)	0.0246 (11)	0.0201 (11)	0.0000 (10)	−0.0009 (9)	−0.0017 (9)
C2'	0.0345 (11)	0.0219 (10)	0.0228 (11)	0.0007 (10)	−0.0003 (10)	−0.0030 (9)

O2'	0.0423 (10)	0.0277 (9)	0.0280 (9)	−0.0076 (8)	0.0058 (8)	−0.0098 (8)
C3'	0.0364 (12)	0.0233 (10)	0.0257 (11)	−0.0026 (10)	0.0032 (11)	−0.0065 (9)
O3'	0.0565 (13)	0.0341 (10)	0.0394 (11)	−0.0134 (10)	0.0207 (10)	−0.0118 (9)
C4'	0.0435 (14)	0.0290 (12)	0.0195 (11)	0.0016 (12)	−0.0015 (10)	−0.0011 (9)
O4'	0.0359 (9)	0.0343 (9)	0.0251 (9)	0.0084 (8)	−0.0018 (8)	0.0004 (7)
C5'	0.0590 (18)	0.0265 (12)	0.0329 (13)	0.0037 (14)	−0.0046 (14)	0.0040 (11)
O5'	0.0514 (12)	0.0286 (10)	0.0512 (14)	0.0065 (10)	−0.0038 (11)	−0.0063 (10)
O1W	0.108 (9)	0.060 (4)	0.080 (4)	0.015 (5)	−0.009 (4)	0.018 (3)
O1W'	0.113 (17)	0.084 (8)	0.146 (13)	−0.011 (9)	−0.050 (13)	0.024 (8)
O2W	0.075 (2)	0.122 (3)	0.0549 (18)	0.036 (2)	−0.0032 (16)	−0.0002 (19)
O3W	0.046 (5)	0.096 (9)	0.178 (14)	0.021 (5)	0.011 (7)	0.008 (10)
O3W'	0.125 (11)	0.108 (9)	0.121 (9)	0.054 (9)	0.045 (8)	0.049 (7)

Geometric parameters (Å, °)

O1—C1	1.223 (3)	C9—H9	0.93
O2—C2	1.240 (3)	C10—H10	0.93
N1—C4	1.372 (3)	C1'—O4'	1.406 (3)
N1—C1	1.380 (3)	C1'—C2'	1.524 (4)
N1—C1'	1.499 (3)	C1'—H1'	0.98
N2—C1	1.368 (3)	C2'—O2'	1.423 (3)
N2—C2	1.380 (3)	C2'—C3'	1.525 (4)
N2—H2	0.86	C2'—H2'	0.98
C2—C3	1.439 (3)	O2'—H2O'	0.82
C3—C4	1.362 (3)	C3'—O3'	1.414 (3)
C3—C5	1.479 (4)	C3'—C4'	1.519 (4)
C4—H4	0.93	C3'—H3'	0.98
C5—C10	1.391 (4)	O3'—H3O'	0.82
C5—C6	1.398 (4)	C4'—O4'	1.447 (3)
C6—C7	1.378 (4)	C4'—C5'	1.499 (4)
C6—H6	0.93	C4'—H4'	0.98
C7—C8	1.389 (6)	C5'—O5'	1.430 (4)
C7—H7	0.93	C5'—H51'	0.97
C8—C9	1.395 (7)	C5'—H52'	0.97
C8—H8	0.93	O5'—H5O'	0.82
C9—C10	1.389 (4)		
C4—N1—C1	121.1 (2)	C5—C10—H10	119.2
C4—N1—C1'	122.6 (2)	O4'—C1'—N1	108.89 (19)
C1—N1—C1'	115.7 (2)	O4'—C1'—C2'	107.0 (2)
C1—N2—C2	127.3 (2)	N1—C1'—C2'	111.9 (2)
C1—N2—H2	116.3	O4'—C1'—H1'	109.7
C2—N2—H2	116.3	N1—C1'—H1'	109.7
O1—C1—N2	122.9 (2)	C2'—C1'—H1'	109.7
O1—C1—N1	122.3 (3)	O2'—C2'—C1'	105.6 (2)
N2—C1—N1	114.8 (2)	O2'—C2'—C3'	110.9 (2)
O2—C2—N2	118.6 (2)	C1'—C2'—C3'	101.4 (2)
O2—C2—C3	125.9 (2)	O2'—C2'—H2'	112.7
N2—C2—C3	115.4 (2)	C1'—C2'—H2'	112.7
C4—C3—C2	117.8 (2)	C3'—C2'—H2'	112.7

C4—C3—C5	120.5 (2)	C2'—O2'—H2O'	109.5
C2—C3—C5	121.7 (2)	O3'—C3'—C4'	113.4 (2)
C3—C4—N1	123.4 (2)	O3'—C3'—C2'	111.9 (2)
C3—C4—H4	118.3	C4'—C3'—C2'	101.8 (2)
N1—C4—H4	118.3	O3'—C3'—H3'	109.8
C10—C5—C6	118.3 (3)	C4'—C3'—H3'	109.8
C10—C5—C3	119.8 (3)	C2'—C3'—H3'	109.8
C6—C5—C3	121.9 (3)	C3'—O3'—H3O'	109.5
C7—C6—C5	120.7 (3)	O4'—C4'—C5'	109.8 (2)
C7—C6—H6	119.7	O4'—C4'—C3'	104.1 (2)
C5—C6—H6	119.7	C5'—C4'—C3'	117.3 (3)
C6—C7—C8	120.7 (4)	O4'—C4'—H4'	108.4
C6—C7—H7	119.7	C5'—C4'—H4'	108.4
C8—C7—H7	119.7	C3'—C4'—H4'	108.4
C7—C8—C9	119.5 (3)	C1'—O4'—C4'	110.48 (19)
C7—C8—H8	120.2	O5'—C5'—C4'	111.8 (2)
C9—C8—H8	120.2	O5'—C5'—H51'	109.2
C10—C9—C8	119.3 (4)	C4'—C5'—H51'	109.2
C10—C9—H9	120.3	O5'—C5'—H52'	109.2
C8—C9—H9	120.3	C4'—C5'—H52'	109.2
C9—C10—C5	121.5 (3)	H51'—C5'—H52'	107.9
C9—C10—H10	119.2	C5'—O5'—H5O'	109.5
C2—N2—C1—O1	177.3 (3)	C8—C9—C10—C5	−0.3 (5)
C2—N2—C1—N1	−3.4 (4)	C6—C5—C10—C9	1.2 (5)
C4—N1—C1—O1	−176.1 (3)	C3—C5—C10—C9	−178.0 (3)
C1'—N1—C1—O1	−4.5 (4)	C4—N1—C1'—O4'	1.7 (3)
C4—N1—C1—N2	4.5 (4)	C1—N1—C1'—O4'	−169.9 (2)
C1'—N1—C1—N2	176.2 (2)	C4—N1—C1'—C2'	−116.3 (3)
C1—N2—C2—O2	−178.6 (3)	C1—N1—C1'—C2'	72.1 (3)
C1—N2—C2—C3	1.5 (4)	O4'—C1'—C2'—O2'	88.5 (2)
O2—C2—C3—C4	179.5 (3)	N1—C1'—C2'—O2'	−152.3 (2)
N2—C2—C3—C4	−0.7 (4)	O4'—C1'—C2'—C3'	−27.3 (2)
O2—C2—C3—C5	0.0 (4)	N1—C1'—C2'—C3'	91.9 (2)
N2—C2—C3—C5	179.8 (2)	O2'—C2'—C3'—O3'	47.3 (3)
C2—C3—C4—N1	2.1 (4)	C1'—C2'—C3'—O3'	159.1 (2)
C5—C3—C4—N1	−178.4 (2)	O2'—C2'—C3'—C4'	−74.2 (2)
C1—N1—C4—C3	−4.2 (4)	C1'—C2'—C3'—C4'	37.6 (2)
C1'—N1—C4—C3	−175.3 (2)	O3'—C3'—C4'—O4'	−155.9 (2)
C4—C3—C5—C10	38.3 (4)	C2'—C3'—C4'—O4'	−35.4 (2)
C2—C3—C5—C10	−142.2 (3)	O3'—C3'—C4'—C5'	82.7 (3)
C4—C3—C5—C6	−140.9 (3)	C2'—C3'—C4'—C5'	−156.9 (2)
C2—C3—C5—C6	38.7 (4)	N1—C1'—O4'—C4'	−115.8 (2)
C10—C5—C6—C7	−1.1 (4)	C2'—C1'—O4'—C4'	5.3 (3)
C3—C5—C6—C7	178.1 (3)	C5'—C4'—O4'—C1'	145.6 (2)
C5—C6—C7—C8	0.2 (5)	C3'—C4'—O4'—C1'	19.3 (3)
C6—C7—C8—C9	0.7 (6)	O4'—C4'—C5'—O5'	−64.2 (3)
C7—C8—C9—C10	−0.6 (6)	C3'—C4'—C5'—O5'	54.2 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3'^{i}	0.86	2.02	2.842 (3)	159
O2'—H2O'···O2^{ii}	0.82	2	2.740 (3)	151
O3'—H3O'···O3W^{iii}	0.82	1.83	2.600 (9)	157
O3'—H3O'···O3W'^{iii}	0.82	1.88	2.691 (9)	169
O5'—H5O'···O2'^{iv}	0.82	1.92	2.735 (3)	171

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

Fig. 1

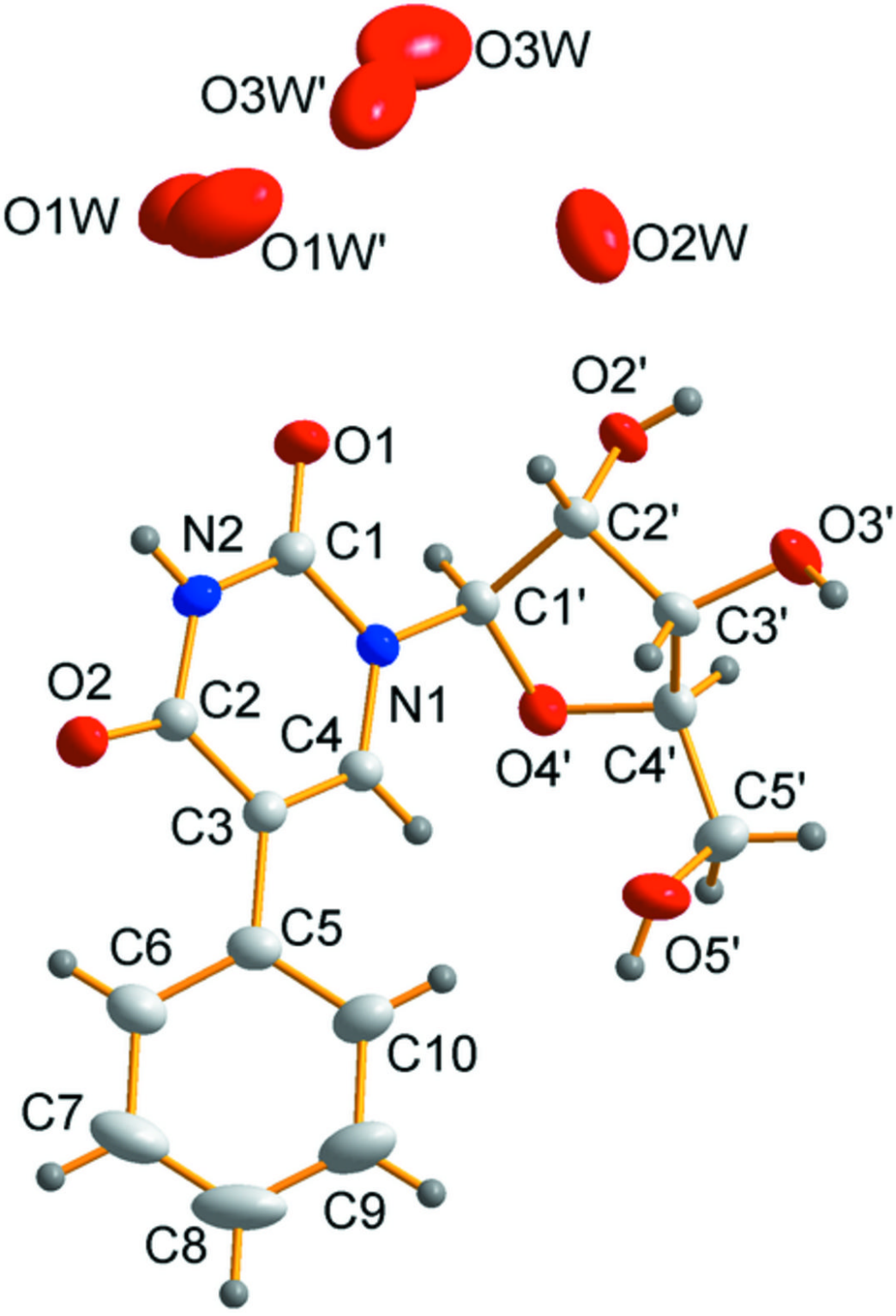
O3W
O3W'
O1W
O1W'
O2W
O2'
O1
C2'
O3'
N2
C1
C1'
C3'
O2
C2
N1
C4
O4'
C4'
C5'
C3
C5
C6
O5'
C10
C7
C9
C8

Fig. 2