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Hydrogen-bonding patterns in bis(cytosinium) tartarate monohydrate

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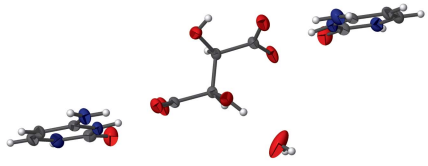
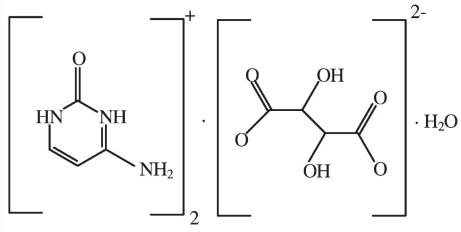
The asymmetric unit of the title cytosinium salt derivative, $2C_4H_6N_3O^+\cdot C4H4O62-\cdot H_2O$, contains two cytosinium cations, one tartaric acid anion and a water molecule. The two cytosinium cations are almost planar (r.m.s. deviations of the fitted atoms are 0.0151 and 0.0213 Å). The crystal structure features C—H···O, N—H···O and O—H···O interactions. Further C—O···π and π–π interactions are observed along the *ab* plane, contributing to the crystal stability.

3D view



Chemical scheme



Structure description

Pyrimidine-based derivatives have attracted a great deal of attention in terms of their hydrogen-bonding patterns. Cytosinium is one of the naturally occurring base molecules found in DNA and RNA (Portalone *et al.*, 2009). Many cytosinium salts of organic acids have been reported previously, *viz*. cytosinium hydrogen sulfate, cytosinium perchlorate (Bensegueni *et al.*, 2009), cytosinium dihydrogen phosphite (Messai *et al.*, 2009), cytosinium hydrogen chloranilate monohydrate (Gotoh *et al.*, 2006) and cytosinium zoledronate trihydrate (Sridhar & Ravikumar, 2011). As part of our investigations on the growth and characterization of semi-organic crystals containing the nucleic acid component cytosine, we report herein the crystal structure determination and the geometry optimization of the title compound.

A perspective view of the title compound with the atomic numbering scheme is illustrated in Fig. 1. It crystallizes in the orthorhombic space group $P2_12_12_1$ with two cytosinium cations, a tartarate anion and one water molecule. The two cytosinium

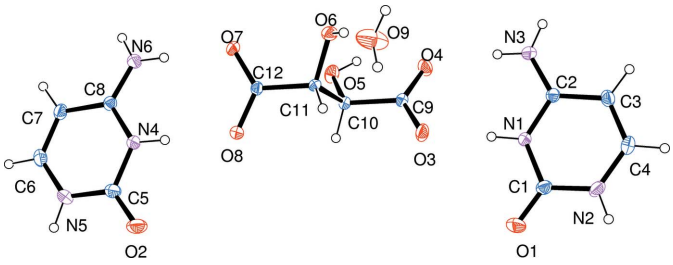


Figure 1
The molecular structure with displacement ellipsoids for the non-H atoms drawn at the 30% probability level.

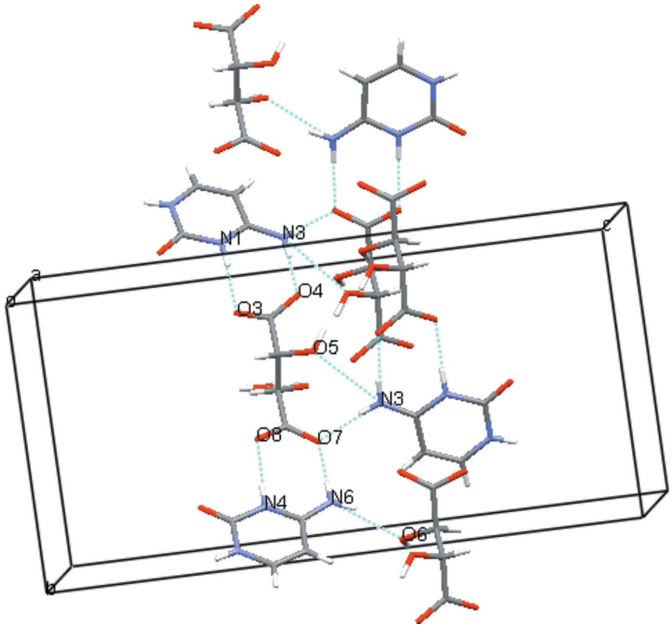


Figure 2
Crystal packing of the title compound, showing the N—H···O interactions in the $R_2^2(12)$ motif along the *c* axis and in parallel chains along the *a* and *c* axes as dashed lines. Other H atoms have been omitted for clarity.

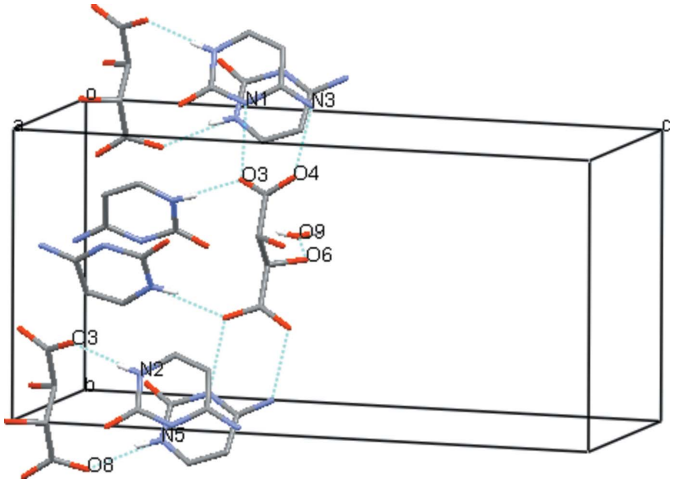


Figure 3
Crystal packing of the title compound, showing the N—H···O interactions enclosing parallel chains along the *c* and *a* axes and O—H···O interactions enclosing parallel chains along the *ab* plane, as dashed lines. Other H atoms have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.53	3.098 (2)	120
C10—H10···O2^{ii}	0.98	2.33	3.312 (2)	175
C11—H11···O1^{iii}	0.98	2.38	3.361 (2)	179
O5—H5···O4	0.82	2.12	2.6140 (19)	118
O6—H6*A*···O9	0.82	1.87	2.688 (2)	172
N1—H1*A*···O3	0.86 (2)	1.80 (2)	2.656 (2)	171 (3)
N2—H2*A*···O3^{i}	0.86 (2)	1.91 (2)	2.768 (2)	175 (3)
N3—H3*A*···O4	0.84 (2)	2.04 (2)	2.873 (2)	171 (2)
N3—H3*B*···O7^{iv}	0.83 (2)	2.04 (2)	2.865 (2)	172 (2)
N4—H4*A*···O8	0.85 (2)	1.90 (2)	2.748 (2)	173 (3)
N5—H5*A*···O8^{v}	0.86 (2)	1.93 (2)	2.766 (2)	166 (3)
N6—H6*B*···O7	0.85 (2)	1.96 (2)	2.808 (2)	179 (3)
N6—H6*C*···O6^{vi}	0.83 (2)	2.01 (2)	2.812 (2)	163 (2)
O9—H9*A*···O2^{i}	0.83 (2)	2.24 (3)	3.040 (3)	162 (4)
O9—H9*B*···O5^{vii}	0.84 (2)	2.00 (3)	2.812 (2)	161 (3)

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

cations are almost planar, the r.m.s deviations of the fitted atoms C1–C4/N1–N3/O1 and C5–C8/N4–N6/O2 being 0.0151 and 0.0213 Å, respectively. An overlay analysis of the two cations gives an r.m.s. deviation of 1.128 Å. Bond distances and angles in the cations are comparable to those in the cation of cytosinium zoledronate trihydrate (Sridhar & Ravikumar, 2011).

The crystal structure features C—H···O, N—H···O and O—H···O interactions. The interaction between N4 and O8 through H4*A*, N6 and O7 through H6*B* and N1 and O3 through H1*A*, N3 and O4 through H3*A* occur alternately as chain links and form a three-dimensional network enclosing $R_2^2(8)$ ring motifs. The interaction between N3 and O7 through H3*B* and N6 and O6 through H6*C* form parallel chains along the *a*- and *c*-axis directions, respectively (Fig. 2). Similarly the interactions between N2 and O3 through H2*A* and N5 and O8 through H5*A* form infinite parallel chains along the *c*- and *a*-axis directions, respectively. The O6—H6*A*···O9 interaction encloses parallel chains along the *ab* plane (Fig. 3). Also the interactions of C4, C11 with O1 through H4, H11 form infinite parallel chains along the *b*- and *c*-axis directions, respectively (Fig. 4). The O9 interactions with O2, O5 through H9*A*, H9*B*

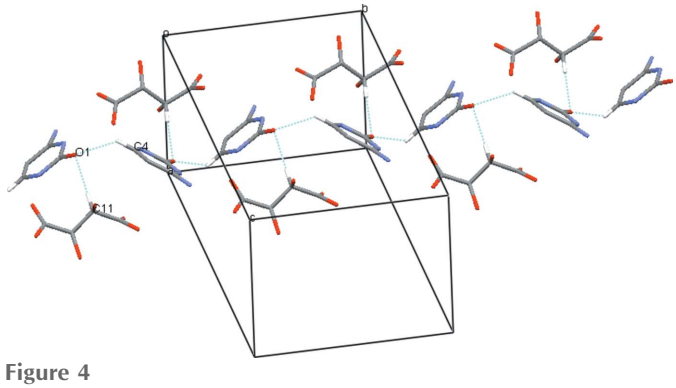


Figure 4
Crystal packing of the title compound, showing the C—H···O interactions enclosing parallel chains along the *b* and *c* axes as dashed lines. Other H atoms have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_4H_6N_3O^+\cdot C_4H_4O_6^{2-}\cdot H_2O$
M_r	390.32
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	7.6932 (8), 10.1152 (8), 20.9336 (17)
V (Å^3)	1629.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.14
Crystal size (mm)	0.25 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan *SADABS*
T_{min}, T_{max}	0.705, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22011, 4920, 4299
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.713
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.087, 1.11
No. of reflections	4920
No. of parameters	284
No. of restraints	13
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.22
Absolute structure	Flack x determined using 1669 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.1 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *XPREP* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Qmol* (Gans & Shalloway, 2001), *Mercury* (Macrae *et al.*, 2008), *ORTEPIII* (Burnett & Johnson, 1996), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

and the interaction between C10 and O2 through H10 forms an $R_3^3(7)$ ring motif along the *ab* plane (Fig. 5). A short contact is observed in the tartarate anion between atoms O4 and O5. Details are given in Table 1.

C—O···π interactions are observed along the *ab* plane [C9···*Cg*2(x, $-1+y$, z) = 3.876 (2) Å, C9—O3···*Cg*2(x, $-1+y$, z) = 15°; C12···*Cg*1(x, $1+y$, z) = 3.497 (2) Å, C12—O8···*Cg*1 = 2°; *Cg*1 and *Cg*2 are the centroids of the N1/C1/N2/C4/C3/C2 and N4/C5/N5/C6/C7/C8 rings, respectively]. In addition, weak π–π interactions are observed between the two symmetry-related cytosinium rings, with *Cg*1···*Cg*2($-1+x$, $-1+y$, z) = 3.401 (2) Å.

Synthesis and crystallization

A hot supersaturated water solution of cytosine (0.111 g, from Spectrochem) and tartaric acid (0.150 g, from Loba Chemie, India) were mixed in a 1:1 molar ratio and the solution was allowed to evaporate slowly, resulting in the formation of transparent plate-like crystals of cytosinium tartrate monohydrate in 15 days (m.p. 491–493 K).

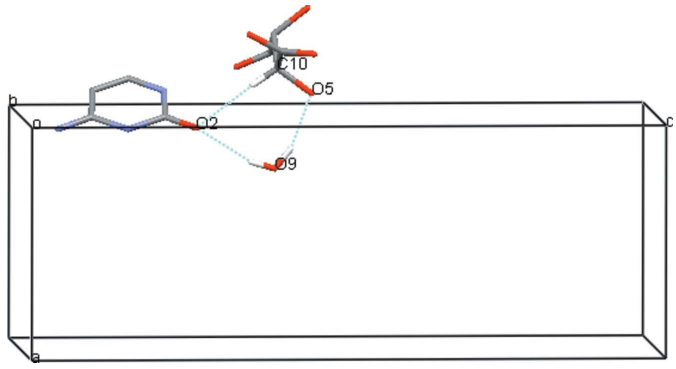


Figure 5
Crystal packing of the title compound, showing the C—H···O and O—H···O interactions enclosing an $R_3^3(7)$ ring motif and parallel chains along the *ab* plane as dashed lines. Other H atoms have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Hydrogen-bonding patterns in bis(cytosinium) tartarate monohydrate

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Bis(cystosinium) tartarate monohydrate

Crystal data

$2C_4H_6N_3O^+\cdot C_4H_4O_6^{2-}\cdot H_2O$
M_r = 390.32
Orthorhombic, $P2_12_12_1$
a = 7.6932 (8) Å
b = 10.1152 (8) Å
c = 20.9336 (17) Å
V = 1629.0 (3) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.592 Mg m^{-3}
Melting point: 493 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7834 reflections
θ = 2.8–28.9°
μ = 0.14 mm^{-1}
T = 296 K
Plate, colourless
0.25 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan SADABS
T_{min} = 0.705, T_{max} = 0.746
22011 measured reflections
4920 independent reflections
4299 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 30.5°, θ_{min} = 2.2°
h = −10→10
k = −14→14
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 1.11
4920 reflections
284 parameters
13 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.2224P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack x determined using 1669 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.1 (3)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5157 (3)	−0.12312 (19)	0.28216 (8)	0.0271 (4)
C2	0.4512 (2)	−0.13171 (17)	0.39524 (8)	0.0227 (3)
C3	0.3533 (3)	−0.24948 (18)	0.38552 (9)	0.0280 (4)
H3	0.3003	−0.2928	0.4195	0.034*
C4	0.3402 (3)	−0.29593 (18)	0.32550 (10)	0.0302 (4)
H4	0.2755	−0.3721	0.3182	0.036*
C5	1.0040 (3)	0.91530 (19)	0.27540 (9)	0.0282 (4)
C6	1.1517 (3)	1.09471 (19)	0.32643 (10)	0.0311 (4)
H6	1.2200	1.1700	0.3220	0.037*
C7	1.1029 (3)	1.05652 (18)	0.38512 (9)	0.0279 (4)
H7	1.1340	1.1050	0.4211	0.033*
C8	1.0018 (2)	0.93903 (17)	0.39043 (8)	0.0228 (3)
C9	0.6955 (2)	0.21335 (16)	0.40007 (8)	0.0223 (3)
C10	0.7829 (2)	0.34860 (16)	0.39920 (8)	0.0205 (3)
H10	0.8548	0.3549	0.3607	0.025*
C11	0.6476 (2)	0.45940 (16)	0.39747 (8)	0.0191 (3)
H11	0.5796	0.4511	0.3581	0.023*
C12	0.7400 (2)	0.59383 (15)	0.39722 (8)	0.0203 (3)
N1	0.5288 (2)	−0.07644 (15)	0.34392 (7)	0.0244 (3)
N2	0.4183 (3)	−0.23531 (17)	0.27525 (8)	0.0313 (4)
N3	0.4693 (3)	−0.07353 (16)	0.45057 (8)	0.0303 (4)
N4	0.9555 (2)	0.87599 (16)	0.33577 (7)	0.0245 (3)
N5	1.1043 (3)	1.02646 (17)	0.27297 (8)	0.0327 (4)
N6	0.9557 (3)	0.88801 (16)	0.44485 (8)	0.0303 (4)
O1	0.5847 (2)	−0.06662 (17)	0.23794 (7)	0.0443 (4)
O2	0.9624 (2)	0.85238 (17)	0.22833 (7)	0.0438 (4)
O3	0.6214 (2)	0.17628 (13)	0.34904 (7)	0.0366 (4)
O4	0.7027 (2)	0.14814 (14)	0.44995 (7)	0.0347 (3)
O5	0.89220 (18)	0.36252 (13)	0.45351 (7)	0.0308 (3)
H5	0.8871	0.2952	0.4752	0.046*
O6	0.53350 (18)	0.44816 (13)	0.45043 (6)	0.0276 (3)
H6A	0.4348	0.4328	0.4376	0.041*
O7	0.74807 (19)	0.65974 (12)	0.44753 (6)	0.0273 (3)
O8	0.8050 (2)	0.63023 (14)	0.34462 (6)	0.0348 (3)
O9	0.2191 (3)	0.4089 (3)	0.39776 (10)	0.0725 (8)
H1A	0.569 (4)	0.003 (2)	0.3477 (12)	0.051 (8)*
H2A	0.403 (3)	−0.258 (3)	0.2363 (9)	0.038 (7)*
H3A	0.529 (3)	−0.004 (2)	0.4530 (11)	0.037 (7)*
H3B	0.411 (3)	−0.094 (2)	0.4827 (9)	0.026 (6)*
H4A	0.902 (3)	0.802 (2)	0.3369 (11)	0.041 (7)*
H5A	1.138 (4)	1.046 (3)	0.2351 (10)	0.044 (7)*
H6B	0.895 (3)	0.8185 (19)	0.4459 (11)	0.036 (7)*
H6C	0.986 (3)	0.921 (2)	0.4795 (9)	0.037 (6)*
H9A	0.190 (5)	0.401 (4)	0.3598 (11)	0.096 (14)*
H9B	0.134 (4)	0.397 (4)	0.4223 (14)	0.088 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0325 (9)	0.0277 (8)	0.0211 (8)	0.0014 (8)	−0.0023 (7)	−0.0016 (7)
C2	0.0259 (8)	0.0190 (7)	0.0232 (7)	0.0033 (7)	0.0007 (7)	0.0005 (6)
C3	0.0308 (10)	0.0211 (8)	0.0323 (10)	−0.0018 (7)	0.0024 (8)	0.0032 (7)
C4	0.0320 (10)	0.0210 (8)	0.0377 (10)	−0.0018 (8)	−0.0044 (8)	−0.0034 (8)
C5	0.0304 (10)	0.0314 (9)	0.0227 (8)	0.0018 (8)	0.0024 (7)	0.0013 (7)
C6	0.0324 (10)	0.0222 (8)	0.0387 (10)	−0.0020 (8)	0.0023 (8)	0.0040 (8)
C7	0.0318 (10)	0.0217 (8)	0.0302 (9)	−0.0028 (8)	−0.0024 (8)	−0.0028 (7)
C8	0.0237 (8)	0.0209 (7)	0.0237 (8)	0.0025 (6)	−0.0011 (6)	0.0002 (7)
C9	0.0280 (9)	0.0174 (7)	0.0217 (8)	−0.0007 (7)	0.0011 (7)	−0.0019 (6)
C10	0.0232 (8)	0.0177 (7)	0.0205 (7)	−0.0020 (6)	0.0006 (6)	−0.0020 (6)
C11	0.0228 (8)	0.0187 (7)	0.0158 (7)	−0.0018 (6)	−0.0009 (6)	−0.0026 (6)
C12	0.0235 (8)	0.0166 (7)	0.0209 (7)	0.0004 (6)	−0.0016 (6)	0.0001 (6)
N1	0.0330 (8)	0.0200 (7)	0.0202 (7)	−0.0036 (6)	0.0005 (6)	−0.0011 (6)
N2	0.0410 (10)	0.0278 (8)	0.0250 (8)	−0.0017 (7)	−0.0048 (7)	−0.0077 (6)
N3	0.0435 (10)	0.0264 (8)	0.0210 (7)	−0.0037 (7)	0.0051 (7)	−0.0014 (6)
N4	0.0287 (8)	0.0225 (7)	0.0223 (7)	−0.0036 (6)	0.0004 (6)	−0.0009 (6)
N5	0.0414 (10)	0.0311 (8)	0.0256 (8)	−0.0027 (7)	0.0056 (7)	0.0065 (7)
N6	0.0422 (10)	0.0278 (8)	0.0210 (7)	−0.0083 (7)	−0.0002 (7)	−0.0018 (6)
O1	0.0591 (11)	0.0519 (10)	0.0219 (6)	−0.0129 (9)	0.0033 (7)	0.0021 (6)
O2	0.0543 (10)	0.0535 (10)	0.0235 (6)	−0.0138 (9)	0.0041 (7)	−0.0069 (7)
O3	0.0632 (11)	0.0226 (6)	0.0241 (6)	−0.0123 (7)	−0.0124 (7)	0.0010 (5)
O4	0.0496 (9)	0.0285 (7)	0.0261 (6)	−0.0091 (7)	−0.0056 (6)	0.0074 (6)
O5	0.0306 (7)	0.0262 (6)	0.0355 (7)	−0.0010 (6)	−0.0120 (6)	−0.0019 (6)
O6	0.0240 (6)	0.0311 (6)	0.0277 (6)	−0.0020 (6)	0.0056 (5)	−0.0044 (5)
O7	0.0398 (8)	0.0208 (6)	0.0212 (6)	−0.0040 (5)	−0.0013 (5)	−0.0042 (5)
O8	0.0563 (10)	0.0249 (6)	0.0233 (6)	−0.0100 (7)	0.0110 (6)	−0.0027 (5)
O9	0.0402 (10)	0.137 (2)	0.0409 (10)	−0.0349 (13)	0.0010 (9)	−0.0080 (13)

Geometric parameters (Å, º)

C1—O1	1.211 (2)	C9—C10	1.524 (2)
C1—N2	1.367 (3)	C10—O5	1.421 (2)
C1—N1	1.380 (2)	C10—C11	1.530 (2)
C2—N3	1.307 (2)	C10—H10	0.9800
C2—N1	1.350 (2)	C11—O6	1.419 (2)
C2—C3	1.424 (3)	C11—C12	1.534 (2)
C3—C4	1.345 (3)	C11—H11	0.9800
C3—H3	0.9300	C12—O7	1.248 (2)
C4—N2	1.358 (3)	C12—O8	1.264 (2)
C4—H4	0.9300	N1—H1A	0.86 (2)
C5—O2	1.216 (2)	N2—H2A	0.857 (18)
C5—N5	1.364 (3)	N3—H3A	0.842 (18)
C5—N4	1.377 (2)	N3—H3B	0.834 (17)
C6—C7	1.341 (3)	N4—H4A	0.854 (19)
C6—N5	1.365 (3)	N5—H5A	0.857 (19)

C6—H6	0.9300	N6—H6B	0.846 (18)
C7—C8	1.425 (3)	N6—H6C	0.833 (17)
C7—H7	0.9300	O5—H5	0.8200
C8—N6	1.300 (2)	O6—H6A	0.8200
C8—N4	1.358 (2)	O9—H9A	0.83 (2)
C9—O4	1.236 (2)	O9—H9B	0.84 (2)
C9—O3	1.267 (2)		

O1—C1—N2	123.44 (18)	C11—C10—H10	108.5
O1—C1—N1	121.52 (18)	O6—C11—C10	110.11 (14)
N2—C1—N1	115.04 (17)	O6—C11—C12	111.12 (13)
N3—C2—N1	118.14 (17)	C10—C11—C12	109.52 (14)
N3—C2—C3	124.05 (17)	O6—C11—H11	108.7
N1—C2—C3	117.81 (16)	C10—C11—H11	108.7
C4—C3—C2	117.74 (18)	C12—C11—H11	108.7
C4—C3—H3	121.1	O7—C12—O8	124.04 (15)
C2—C3—H3	121.1	O7—C12—C11	119.58 (15)
C3—C4—N2	122.18 (18)	O8—C12—C11	116.38 (15)
C3—C4—H4	118.9	C2—N1—C1	124.84 (16)
N2—C4—H4	118.9	C2—N1—H1A	118.0 (18)
O2—C5—N5	123.37 (18)	C1—N1—H1A	115.5 (18)
O2—C5—N4	121.41 (18)	C4—N2—C1	122.35 (16)
N5—C5—N4	115.20 (17)	C4—N2—H2A	123.5 (17)
C7—C6—N5	122.05 (18)	C1—N2—H2A	113.8 (17)
C7—C6—H6	119.0	C2—N3—H3A	119.2 (16)
N5—C6—H6	119.0	C2—N3—H3B	123.3 (15)
C6—C7—C8	117.66 (18)	H3A—N3—H3B	117 (2)
C6—C7—H7	121.2	C8—N4—C5	124.52 (16)
C8—C7—H7	121.2	C8—N4—H4A	121.0 (16)
N6—C8—N4	118.70 (16)	C5—N4—H4A	114.1 (16)
N6—C8—C7	123.27 (17)	C5—N5—C6	122.51 (17)
N4—C8—C7	118.01 (16)	C5—N5—H5A	113.3 (18)
O4—C9—O3	125.05 (17)	C6—N5—H5A	124.2 (18)
O4—C9—C10	117.97 (16)	C8—N6—H6B	120.2 (16)
O3—C9—C10	116.98 (15)	C8—N6—H6C	121.8 (16)
O5—C10—C9	109.89 (14)	H6B—N6—H6C	118 (2)
O5—C10—C11	110.42 (13)	C10—O5—H5	109.5
C9—C10—C11	110.95 (14)	C11—O6—H6A	109.5
O5—C10—H10	108.5	H9A—O9—H9B	111 (3)
C9—C10—H10	108.5		

N3—C2—C3—C4	177.53 (19)	O6—C11—C12—O8	−160.68 (16)
N1—C2—C3—C4	−1.9 (3)	C10—C11—C12—O8	77.45 (19)
C2—C3—C4—N2	0.9 (3)	N3—C2—N1—C1	−177.22 (18)
N5—C6—C7—C8	1.4 (3)	C3—C2—N1—C1	2.3 (3)
C6—C7—C8—N6	175.8 (2)	O1—C1—N1—C2	177.9 (2)
C6—C7—C8—N4	−2.5 (3)	N2—C1—N1—C2	−1.4 (3)
O4—C9—C10—O5	13.0 (2)	C3—C4—N2—C1	0.1 (3)

O3—C9—C10—O5	−166.62 (16)	O1—C1—N2—C4	−179.1 (2)
O4—C9—C10—C11	−109.38 (19)	N1—C1—N2—C4	0.1 (3)
O3—C9—C10—C11	71.0 (2)	N6—C8—N4—C5	−176.22 (18)
O5—C10—C11—O6	−65.06 (17)	C7—C8—N4—C5	2.2 (3)
C9—C10—C11—O6	57.03 (17)	O2—C5—N4—C8	177.85 (19)
O5—C10—C11—C12	57.41 (17)	N5—C5—N4—C8	−0.6 (3)
C9—C10—C11—C12	179.50 (14)	O2—C5—N5—C6	−179.1 (2)
O6—C11—C12—O7	19.7 (2)	N4—C5—N5—C6	−0.6 (3)
C10—C11—C12—O7	−102.17 (18)	C7—C6—N5—C5	0.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.53	3.098 (2)	120
C10—H10···O2^{ii}	0.98	2.33	3.312 (2)	175
C11—H11···O1^{iii}	0.98	2.38	3.361 (2)	179
O5—H5···O4	0.82	2.12	2.6140 (19)	118
O6—H6*A*···O9	0.82	1.87	2.688 (2)	172
N1—H1*A*···O3	0.86 (2)	1.80 (2)	2.656 (2)	171 (3)
N2—H2*A*···O3^{i}	0.86 (2)	1.91 (2)	2.768 (2)	175 (3)
N3—H3*A*···O4	0.84 (2)	2.04 (2)	2.873 (2)	171 (2)
N3—H3*B*···O7^{iv}	0.83 (2)	2.04 (2)	2.865 (2)	172 (2)
N4—H4*A*···O8	0.85 (2)	1.90 (2)	2.748 (2)	173 (3)
N5—H5*A*···O8^{v}	0.86 (2)	1.93 (2)	2.766 (2)	166 (3)
N6—H6*B*···O7	0.85 (2)	1.96 (2)	2.808 (2)	179 (3)
N6—H6*C*···O6^{vi}	0.83 (2)	2.01 (2)	2.812 (2)	163 (2)
O9—H9*A*···O2^{i}	0.83 (2)	2.24 (3)	3.040 (3)	162 (4)
O9—H9*B*···O5^{vii}	0.84 (2)	2.00 (3)	2.812 (2)	161 (3)

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