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Crystal structure of 1*H*,1′*H*-[2,2′-biimidazol]-3-ium hydrogen tartrate hemihydrate

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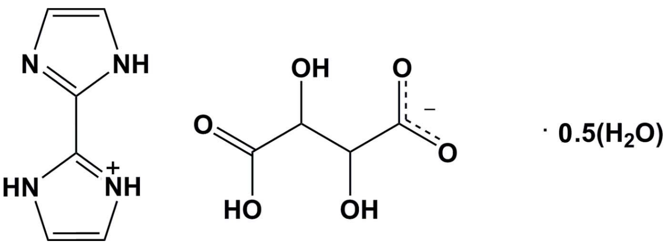
In the crystal of the title hydrated salt, $C_6H_7N_4^+ \cdot C_4H_5O_6^- \cdot 0.5H_2O$, the biimidazole monocation, 1*H*,1′*H*-[2,2′-biimidazol]-3-ium, is hydrogen bonded, *via* N—H⋯O, O—H⋯O and O—H⋯N hydrogen bonds, to the hydrogen tartrate anion and the water molecule, which is located on a twofold rotation axis, forming sheets parallel to (001). The sheets are linked *via* C—H⋯O hydrogen bonds, forming a three-dimensional structure. There are also C═O⋯π interactions present [O⋯π distances are 3.00 (9) and 3.21 (7) Å], involving the carbonyl O atoms and the imidazolium ring, which may help to consolidate the structure. In the cation, the dihedral angle between the rings is 11.6 (2)°.

Keywords: crystal structure; biimidazole; imidazolium; tartrate; hydrogen bonding.

CCDC reference: 1031345

1. Related literature

For background to the use of 2,2′-biimidazoles in crystal engineering, see: Shankar *et al.* (2013); Gulbransen & Fitchett (2012); Tadokoro & Nakasuji (2000). For similar structures, see: Liu & Zhu (2010); Gao *et al.* (2009); Li & Yang (2006); Mori & Miyoshi (2004).



2. Experimental

2.1. Crystal data

$C_4H_5O_6^- \cdot C_6H_7N_4^+ \cdot 0.5H_2O$
M_r = 293.25
Monoclinic, *C*2
a = 19.3211 (13) Å
b = 4.8198 (2) Å
c = 16.1795 (10) Å
β = 122.694 (7)°
V = 1267.99 (13) $Å^3$
Z = 4
Mo *K*α radiation
μ = 0.13 mm^{-1}
T = 296 K
0.35 × 0.30 × 0.23 mm

2.2. Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.956, T_{max} = 0.971
4238 measured reflections
2292 independent reflections
2100 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.099
S = 1.11
2292 reflections
202 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.27 e $Å^{-3}$

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2*A*⋯O2^{i}	0.92 (3)	1.78 (3)	2.683 (3)	169 (3)
N3—H3*A*⋯O5^{ii}	0.94 (3)	1.81 (3)	2.729 (3)	167 (3)
N4—H4*A*⋯O1^{i}	0.91 (3)	1.73 (3)	2.630 (3)	167 (3)
O3—H3⋯O7	0.83	2.05	2.871 (2)	168
O4—H4⋯O3^{iii}	0.91 (4)	1.86 (4)	2.761 (3)	175 (3)
O6—H6*A*⋯N1^{iv}	0.82	1.79	2.598 (3)	168
O7—H7*A*⋯O1	0.93	2.19	2.802 (2)	123
C2—H2⋯O2^{v}	0.93	2.35	3.215 (3)	154
C5—H5⋯O4^{vi}	0.93	2.55	3.415 (3)	155
C6—H6⋯O5^{vii}	0.93	2.37	3.205 (3)	149

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: pubCIF (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5001).

References

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, X.-L., Lu, L.-P. & Zhu, M.-L. (2009). *Acta Cryst.* C**65**, o123–o127.
Gulbransen, J. L. & Fitchett, C. M. (2012). *CrystEngComm*, **14**, 5394–5397.

Li, Y.-P. & Yang, P. (2006). *Acta Cryst.* E**62**, o3223–o3224.

Liu, X. & Zhu, W. (2010). *Acta Cryst.* E**66**, o1245.

Mori, H. & Miyoshi, E. (2004). *Bull. Chem. Soc. Jpn*, **77**, 687–690.

Shankar, B., Elumalai, P., Hussain, F. & Sathiyendiran, M. (2013). *J. Organomet. Chem.* **732**, 130–136.

Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Tadokoro, M. & Nakasuji, K. (2000). *Coord. Chem. Rev.* **198**, 205–218.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

o1222 Gao *et al.* • $C_4H_5O_6^-\cdot C_6H_7N_4^+\cdot 0.5H_2O$ *Acta Cryst.* (2014). E**70**, o1221–o1222

supporting information

Acta Cryst. (2014). E**70**, o1221–o1222 [doi:10.1107/S160053681402371X]

Crystal structure of 1*H*,1′*H*-[2,2′-biimidazol]-3-ium hydrogen tartrate hemihydrate

Xiao-Li Gao, Li-Fang Bian and Shao-Wei Guo

S1. Synthesis and crystallization

Diimidazole (1.0 mmol) and tartaric acid (1.0 mmol) were dissolved in water (15 ml) by adding 1.2 ml of 2M HCl while stirring. The solution was left to stand at room temperature and colourless crystals of the title compound were obtained after several weeks.

S1.1. Refinement

The NH H atoms and the water molecule H atom were located in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(N,O). The O and C bound H atoms were placed in geometrically idealized positions with C—H = 0.93Å and O—H = 0.84 Å and constrained to refine with U_{iso}(H) = 1.2U_{eq}(O,C).

S2. Comment

Supramolecular assemblies built by means of hydrogen bonding interactions have provided numerous materials with very attractive properties (Gulbransen & Fitchett, 2012; Shankar *et al.*, 2013). 2,2′-Biimidazole, H_2biim, is not only a proton donor, but also a proton acceptor, so that it possesses five possible forms, viz. diprotonated (dication, H_4biim^{2+}), monoprotonated (monocation, H_3biim^{+}), dideprotonated (dianion, biim^{2-}), monodeprotonated (monoanion, Hbiim^{-}) (Tadokoro & Nakasuji, 2000; Mori & Miyoshi, 2004). Therefore, H_2biim appears as an interesting molecular building block for the design of new multidimensional supramolecular arrangements, owing to its capacity to act as a donor or acceptor in the formation of hydrogen bonds (Li & Yang, 2006; Gao *et al.*, 2009; Liu & Zhu, 2010).

The fundamental asymmetric unit of compound (I), contains two monoprotonated biimidazolium cations, two tatrate anions and one water molecular, in which the two imidazole rings of biimidazole are little tortile with the dihedral number is 11.5°. Strong N—H···O and O—H···N hydrogen bonds link neighbour tatrate and biimidazolium moities, then O—H···O hydrogen bonds between water molecular and tatrates link them to form two different zigzag layers as shown in Fig. 1. Two groups of these parallel layers on a twofold rotation axis and invension centre forming a zigzag conformation, then further assemble to tapes *via* weak C=O···*π* (centroid of imidazolium ring) interaction arranged alternatively in three-dimensional structure as described in Table 1 and shown in Fig. 2.

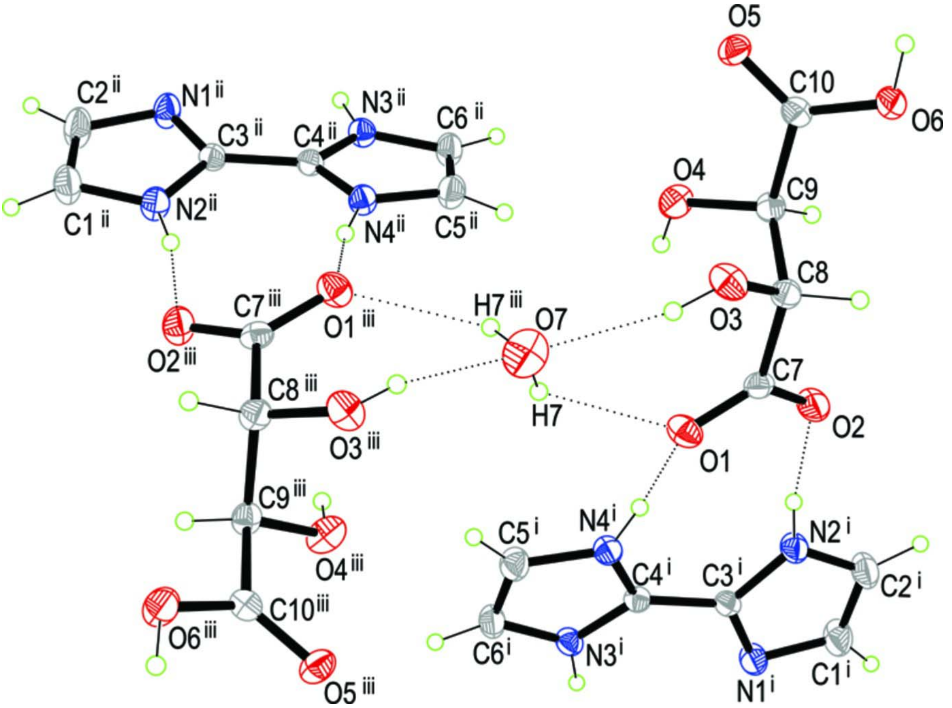

Figure 1

Molecular structure and atom labelling of the title compound, with displacement ellipsoids drawn at the 30% probability level. Dashed line indicates hydrogen bonds [see Table 1 for details; symmetry codes: (i) *x*, *y* + 1, *z*; (ii) *x* + 3/2, *y* + 3/2, *z* + 2; (iii) *x* + 3/2, *y* + 1/2, *z* + 2].

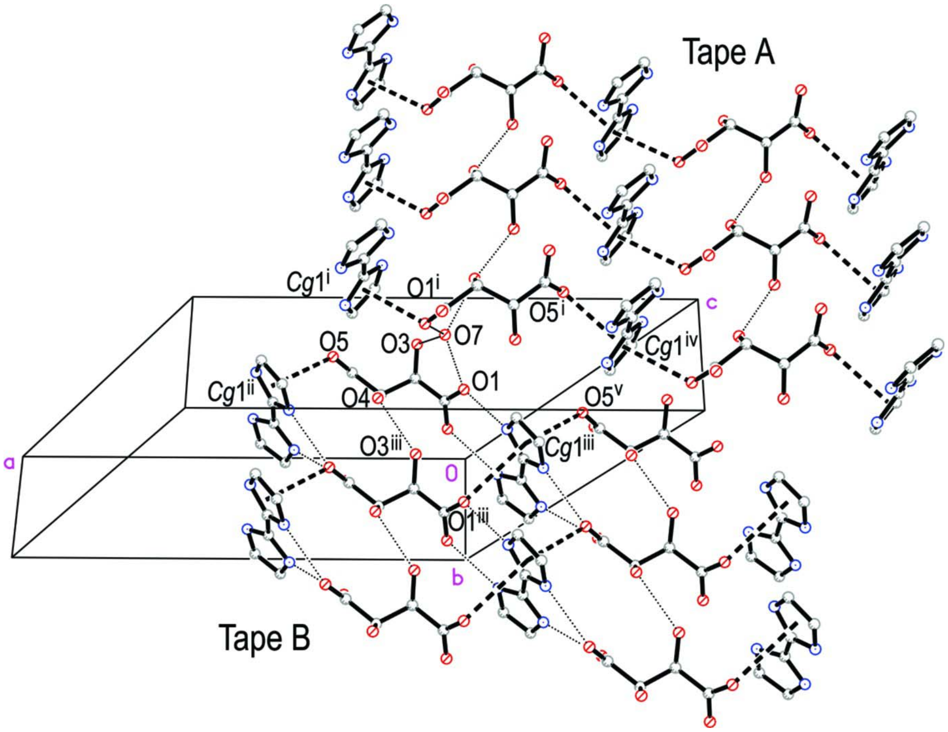

Figure 2

Partial crystal packing of the title compound, with the hydrogen bonds (dashed lines) and C═O···π interactions (dashed solid lines) between neighbouring tapes. Cg1 is the centroid of the C4/C5/C6/N3/N4 imidazole ring. [Symmetry codes: (i) $x + 3/2, y + 1/2, z + 2$; (ii) $-x, y, -z$; (iii) $x, y + 1, z$; (iv) $x + 3/2, y - 3/2, z + 2$; (v) $-x - 1, y, -z$.]

1*H*,1′*H*-[2,2′-Biimidazol]-3-ium 3-carboxy-2,3-dihydroxypropanoate hemihydrate

Crystal data

$C_4H_5O_6^-\cdot C_6H_7N_4^+\cdot 0.5H_2O$
$M_r = 293.25$
Monoclinic, *C*2
Hall symbol: C 2y
$a = 19.3211$ (13) Å
$b = 4.8198$ (2) Å
$c = 16.1795$ (10) Å
$\beta = 122.694$ (7)°
$V = 1267.99$ (13) Å^3
$Z = 4$

$F(000) = 612$
$D_x = 1.536$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2195 reflections
$\theta = 3.5$–25.0°
$\mu = 0.13$ mm^{-1}
$T = 296$ K
Plate, colourless
0.35 × 0.30 × 0.23 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0733 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.956$, $T_{max} = 0.971$

4238 measured reflections
2292 independent reflections
2100 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.6°$
$h = -23 \rightarrow 10$
$k = -5 \rightarrow 5$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.099$
$S = 1.11$
2292 reflections
202 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.5619P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.27$ e Å^{-3}

Special details

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 $F^2 > \sigma(F^2)$ 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.
The line _refine_ls_abs_structure_Flack -1.5 (15) has been removed. According to the comment in an absolute configuration has been assigned, obtained using x by least-squares refinement. There is too high standard uncertainty on x and no information available that the assigned value is confirmed by the diffraction measurements.

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.12363 (19)	0.3256 (7)	0.54798 (19)	0.0501 (8)
H1	0.0811	0.4221	0.4950	0.060*
C2	0.17427 (17)	0.1439 (8)	0.54276 (19)	0.0465 (8)
H2	0.1729	0.0925	0.4865	0.056*
C3	0.20830 (14)	0.1770 (6)	0.69462 (16)	0.0287 (6)
C4	0.25343 (14)	0.1445 (5)	0.80032 (16)	0.0266 (5)
C5	0.33858 (17)	−0.0022 (6)	0.95007 (19)	0.0385 (7)
H5	0.3788	−0.1057	1.0029	0.046*
C6	0.29783 (17)	0.2162 (6)	0.95549 (18)	0.0380 (7)
H6	0.3044	0.2923	1.0121	0.046*
N1	0.14434 (14)	0.3465 (5)	0.64335 (15)	0.0400 (6)
N2	0.22801 (13)	0.0497 (5)	0.63601 (15)	0.0357 (5)
N3	0.24455 (13)	0.3045 (5)	0.86056 (14)	0.0307 (5)
N4	0.31045 (13)	−0.0455 (5)	0.85300 (15)	0.0307 (5)
H2A	0.2689 (17)	−0.079 (6)	0.6544 (19)	0.037*
H3A	0.2032 (17)	0.440 (6)	0.8388 (18)	0.037*
H4A	0.3337 (16)	−0.172 (7)	0.8333 (19)	0.037*
C7	0.38284 (14)	0.5315 (5)	0.74083 (18)	0.0295 (6)
C8	0.44290 (15)	0.3252 (6)	0.74053 (18)	0.0308 (6)
C9	0.51381 (14)	0.4868 (5)	0.74572 (17)	0.0288 (6)
H9	0.4916	0.6076	0.6881	0.035*
C10	0.57380 (15)	0.2829 (6)	0.74598 (17)	0.0299 (6)

O1	0.37823 (11)	0.5416 (4)	0.81509 (13)	0.0379 (5)
O2	0.34295 (11)	0.6789 (4)	0.66602 (12)	0.0436 (5)
O3	0.47460 (11)	0.1317 (4)	0.81901 (13)	0.0382 (5)
H3	0.4744	0.1836	0.8679	0.046*
O4	0.55700 (11)	0.6495 (4)	0.83171 (14)	0.0402 (5)
O5	0.64334 (10)	0.2498 (4)	0.81780 (12)	0.0353 (5)
O6	0.54328 (11)	0.1477 (5)	0.66429 (13)	0.0475 (5)
H6A	0.5803	0.0673	0.6635	0.057*
H4	0.5313 (19)	0.807 (8)	0.832 (2)	0.057*
H8	0.4108 (19)	0.231 (7)	0.676 (2)	0.057*
O7	0.5000	0.3371 (9)	1.0000	0.0714 (10)
H7A	0.4667	0.4934	0.9729	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0480 (17)	0.063 (2)	0.0286 (13)	0.0215 (17)	0.0139 (13)	0.0062 (15)
C2	0.0506 (17)	0.0589 (19)	0.0278 (13)	0.0134 (17)	0.0196 (12)	0.0000 (14)
C3	0.0276 (12)	0.0321 (13)	0.0280 (12)	0.0028 (12)	0.0161 (10)	0.0002 (12)
C4	0.0262 (12)	0.0257 (12)	0.0282 (11)	0.0020 (11)	0.0149 (10)	0.0017 (11)
C5	0.0380 (14)	0.0426 (16)	0.0297 (13)	0.0072 (13)	0.0149 (11)	0.0046 (12)
C6	0.0405 (15)	0.0437 (17)	0.0273 (12)	0.0023 (13)	0.0168 (12)	−0.0015 (12)
N1	0.0373 (12)	0.0501 (14)	0.0286 (11)	0.0179 (12)	0.0152 (10)	0.0038 (11)
N2	0.0348 (12)	0.0400 (13)	0.0305 (11)	0.0110 (11)	0.0165 (10)	−0.0011 (10)
N3	0.0327 (11)	0.0322 (12)	0.0293 (11)	0.0050 (10)	0.0180 (9)	0.0005 (9)
N4	0.0318 (11)	0.0310 (12)	0.0295 (11)	0.0067 (10)	0.0167 (9)	0.0033 (9)
C7	0.0245 (12)	0.0283 (13)	0.0354 (13)	−0.0009 (11)	0.0160 (10)	−0.0059 (11)
C8	0.0300 (13)	0.0297 (14)	0.0312 (12)	0.0041 (11)	0.0155 (11)	−0.0018 (11)
C9	0.0299 (12)	0.0254 (13)	0.0286 (12)	0.0069 (11)	0.0141 (10)	0.0028 (11)
C10	0.0322 (13)	0.0296 (13)	0.0318 (13)	−0.0007 (11)	0.0198 (12)	−0.0003 (11)
O1	0.0442 (11)	0.0357 (10)	0.0423 (10)	0.0090 (9)	0.0290 (9)	0.0043 (8)
O2	0.0412 (11)	0.0545 (13)	0.0332 (9)	0.0233 (11)	0.0190 (8)	0.0074 (10)
O3	0.0501 (11)	0.0284 (10)	0.0445 (10)	0.0103 (9)	0.0311 (9)	0.0066 (9)
O4	0.0355 (10)	0.0283 (9)	0.0462 (10)	0.0036 (9)	0.0151 (8)	−0.0117 (9)
O5	0.0268 (9)	0.0365 (10)	0.0347 (9)	0.0052 (8)	0.0114 (8)	−0.0045 (8)
O6	0.0349 (10)	0.0641 (14)	0.0352 (9)	0.0139 (10)	0.0135 (8)	−0.0140 (10)
O7	0.064 (2)	0.078 (3)	0.061 (2)	0.000	0.0266 (18)	0.000

Geometric parameters (Å, º)

C1—C2	1.350 (4)	N4—H4A	0.91 (3)
C1—N1	1.373 (3)	C7—O2	1.247 (3)
C1—H1	0.9300	C7—O1	1.253 (3)
C2—N2	1.367 (3)	C7—C8	1.530 (4)
C2—H2	0.9300	C8—O3	1.421 (3)
C3—N1	1.333 (3)	C8—C9	1.538 (4)
C3—N2	1.346 (3)	C8—H8	0.99 (3)
C3—C4	1.449 (3)	C9—O4	1.412 (3)

C4—N3	1.325 (3)	C9—C10	1.518 (3)
C4—N4	1.328 (3)	C9—H9	0.9800
C5—C6	1.346 (4)	C10—O5	1.222 (3)
C5—N4	1.372 (3)	C10—O6	1.295 (3)
C5—H5	0.9300	O3—H3	0.8309
C6—N3	1.375 (3)	O4—H4	0.91 (4)
C6—H6	0.9300	O6—H6A	0.8200
N2—H2A	0.92 (3)	O7—H7A	0.9324
N3—H3A	0.94 (3)		

C2—C1—N1	109.7 (2)	C4—N4—C5	107.9 (2)
C2—C1—H1	125.2	C4—N4—H4A	129.2 (17)
N1—C1—H1	125.2	C5—N4—H4A	122.4 (17)
C1—C2—N2	106.9 (2)	O2—C7—O1	125.6 (2)
C1—C2—H2	126.6	O2—C7—C8	116.0 (2)
N2—C2—H2	126.6	O1—C7—C8	118.4 (2)
N1—C3—N2	111.2 (2)	O3—C8—C7	112.7 (2)
N1—C3—C4	124.5 (2)	O3—C8—C9	110.02 (19)
N2—C3—C4	124.3 (2)	C7—C8—C9	109.0 (2)
N3—C4—N4	108.8 (2)	O3—C8—H8	111 (2)
N3—C4—C3	124.8 (2)	C7—C8—H8	105.0 (19)
N4—C4—C3	126.4 (2)	C9—C8—H8	108.7 (18)
C6—C5—N4	108.0 (2)	O4—C9—C10	108.24 (19)
C6—C5—H5	126.0	O4—C9—C8	111.7 (2)
N4—C5—H5	126.0	C10—C9—C8	109.19 (19)
C5—C6—N3	106.3 (2)	O4—C9—H9	109.2
C5—C6—H6	126.8	C10—C9—H9	109.2
N3—C6—H6	126.8	C8—C9—H9	109.2
C3—N1—C1	105.3 (2)	O5—C10—O6	124.4 (2)
C3—N2—C2	106.9 (2)	O5—C10—C9	122.2 (2)
C3—N2—H2A	126.9 (17)	O6—C10—C9	113.4 (2)
C2—N2—H2A	126.1 (17)	C8—O3—H3	115.5
C4—N3—C6	109.0 (2)	C9—O4—H4	116 (2)
C4—N3—H3A	123.3 (16)	C10—O6—H6A	109.5
C6—N3—H3A	127.3 (16)		

N1—C1—C2—N2	−0.3 (4)	N3—C4—N4—C5	−0.2 (3)
N1—C3—C4—N3	−9.7 (4)	C3—C4—N4—C5	179.2 (3)
N2—C3—C4—N3	166.9 (3)	C6—C5—N4—C4	0.1 (3)
N1—C3—C4—N4	170.9 (3)	O2—C7—C8—O3	−169.2 (2)
N2—C3—C4—N4	−12.4 (4)	O1—C7—C8—O3	11.6 (3)
N4—C5—C6—N3	0.1 (3)	O2—C7—C8—C9	68.4 (3)
N2—C3—N1—C1	−0.6 (3)	O1—C7—C8—C9	−110.8 (3)
C4—C3—N1—C1	176.5 (3)	O3—C8—C9—O4	−64.0 (2)
C2—C1—N1—C3	0.5 (4)	C7—C8—C9—O4	60.0 (2)
N1—C3—N2—C2	0.4 (3)	O3—C8—C9—C10	55.7 (3)
C4—C3—N2—C2	−176.7 (3)	C7—C8—C9—C10	179.7 (2)
C1—C2—N2—C3	0.0 (4)	O4—C9—C10—O5	9.8 (3)

N4—C4—N3—C6	0.3 (3)	C8—C9—C10—O5	−112.0 (3)
C3—C4—N3—C6	−179.1 (3)	O4—C9—C10—O6	−171.4 (2)
C5—C6—N3—C4	−0.3 (3)	C8—C9—C10—O6	66.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.92 (3)	1.78 (3)	2.683 (3)	169 (3)
N3—H3*A*···O5^{ii}	0.94 (3)	1.81 (3)	2.729 (3)	167 (3)
N4—H4*A*···O1^{i}	0.91 (3)	1.73 (3)	2.630 (3)	167 (3)
O3—H3···O7	0.83	2.05	2.871 (2)	168
O4—H4···O3^{iii}	0.91 (4)	1.86 (4)	2.761 (3)	175 (3)
O6—H6*A*···N1^{iv}	0.82	1.79	2.598 (3)	168
O7—H7*A*···O1	0.93	2.19	2.802 (2)	123
C2—H2···O2^{v}	0.93	2.35	3.215 (3)	154
C5—H5···O4^{vi}	0.93	2.55	3.415 (3)	155
C6—H6···O5^{vii}	0.93	2.37	3.205 (3)	149

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