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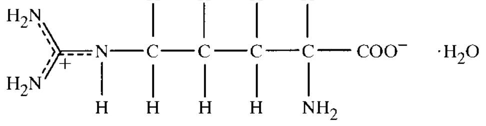
In the title compound, $C_6H_{14}N_4O_2·H_2O$, the α-amino group is neutral. The molecular side chain including the guanidinium group is not fully extended, having a near *gauche–gauche* conformation [χ^3 = 59.0 (1)°; χ^4 = 72.8 (1)°]. The network of hydrogen bonds stabilizing the crystal lattice includes those formed between the deprotonated and negatively charged α-carboxylate groups and the positively charged amino groups of the guanidinium group of neighbouring molecules. N—H···O═C and water-mediated N—H···O hydrogen bonds link individual molecules to produce pairs of spiral motifs laterally connected by N—H···O and C—H···O hydrogen bonds.

Comment

In conjunction with our work of comparative charge-density studies on different amino acids at low temperature by X-ray diffraction methods (Flaig *et al.*, 1999), we crystallized DL-arginine monohydrate, (I), whose structure had not yet been investigated. Arginine is one of the 20 naturally occurring amino acids. It is found in large amounts in protamines and histones. High concentrations of free arginine are also found in many plants including red algae, Cucurbitaceae and conifers, where it serves as a nitrogen storage and transport form. For this reason, it is found in particularly high concentrations in seedlings and reserve organs like rat liver. Young rats and chickens require the amino acid and show stunted growth when fed arginine-free diets because they cannot synthesize it in adequate amounts (Scott & Brewer, 1983).



(I)

Various complexes involving arginine have been investigated by X-ray and neutron techniques, with the Cambridge Structural Database (Allen & Kennard, 1993) containing over 50 entries. Only two crystalline forms involving hydrated free arginine are known: L-arginine dihydrate at room temperature from both X-ray (Karle & Karle, 1964) and neutron diffraction (Lehmann *et al.*, 1973), and DL-arginine dihydrate (Suresh *et al.*, 1994).

An *ORTEP*III (Burnett & Johnson, 1996) representation of the molecular structure of the title compound with the atomic numbering scheme is shown in Fig. 1. The molecule exists as a zwitterion in the crystal structure, the α-carboxylic group is deprotonated and the proton resides in one of the two amino groups of the mesomeric guanidinium fragment. This arrangement permits the formation of two direct N—H···O hydrogen bonds (N3—H71···O1^{iii} and N4—H81···O2^{iii}) (for numbering and symmetry codes of hydrogen bonds see Table 2) between the polar guanidinium and carboxylate groups. This results in a dimeric unit formed by the reference molecule and one generated by the symmetry operation (iii). Each dimer is further linked to other dimeric units by their polar ends, forming an infinite chain of molecules of the same chirality. On the other hand, dimers are interconnected by N4—H82···O1^{v} and C3—H4···O2^{i}. Finally, a pair of these chains is bonded directly by N2—H10···O1^{ii} and indirectly *via* water molecules leading to an infinite three-dimensional lattice.

This arrangement permits the formation of two direct N—H···O hydrogen bonds (N3—H71···O1^{iii} and N4—H81···O2^{iii}; see Fig. 2 and Table 2) between these polar groups. Similar hydrogen-bonding schemes have been observed in L-arginine dihydrate (Karle & Karle, 1964; Lehmann *et al.*, 1973) and DL-arginine dihydrate (Suresh *et al.*, 1994) which also have a neutral α-amino group. This pattern differs from that previously observed for some arginine complexes [L-arginine phosphate monohydrate (Espinosa *et al.*, 1996), DL-arginine formate dihydrate and L-arginine formate (Suresh *et al.*, 1994), DL-arginine DL-glutamate monohydrate and DL-arginine DL-aspartate (Soman *et al.*, 1990)] and crystalline complexes of some peptides [L-arginine

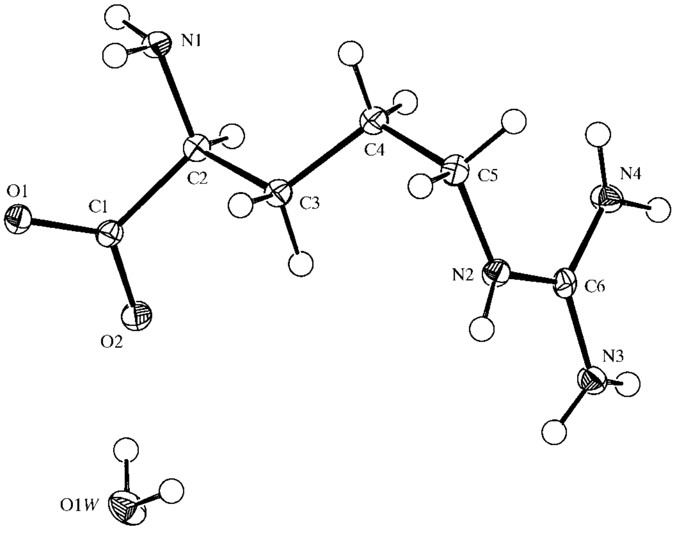


Figure 1
The molecular structure and numbering scheme of the title compound. Displacement ellipsoids are plotted at the 50% probability level (*ORTEP*III; Burnett & Johnson, 1996 and *PLATON*; Spek, 1990).

L-glutamate (Bhat & Vijayan, 1977)] and α-helical peptides (Karle & Balaram, 1990), where the carboxylate group bonds to the protonated α-amino group and not to the guanidinium group. The former sequence is described as having head-to-tail hydrogen bonding (Karle & Balaram, 1990). Unlike L-arginine dihydrate and DL-arginine dihydrate, where the α-amino group does not contribute to N—H···O hydrogen bonding, in (I), one of the H atoms of the α-amino group is donor to an O atom of a solvent water molecule (N1—H2···O1*W*$^{\rm i}$). The observed lack of hydrogen-bond acceptor atoms for H3 of the α-amino group is not surprising. In L-arginine dihydrate (Karle & Karle, 1964; Lehmann *et al.*, 1973) and DL-arginine dihydrate (Suresh *et al.*, 1994), neither α-amino H atom forms a hydrogen bond. Another difference between (I) and the dihydrates is the hydrogen-bonding environment around the guanidinium atom N2. Here, the N—H···N interactions involving these atoms in L-arginine dihydrate and DL-arginine dihydrate (Lehmann *et al.*, 1973; Suresh *et al.*, 1994) are replaced by N—H···O hydrogen bonding: N2—H10···O1$^{\rm i}$.

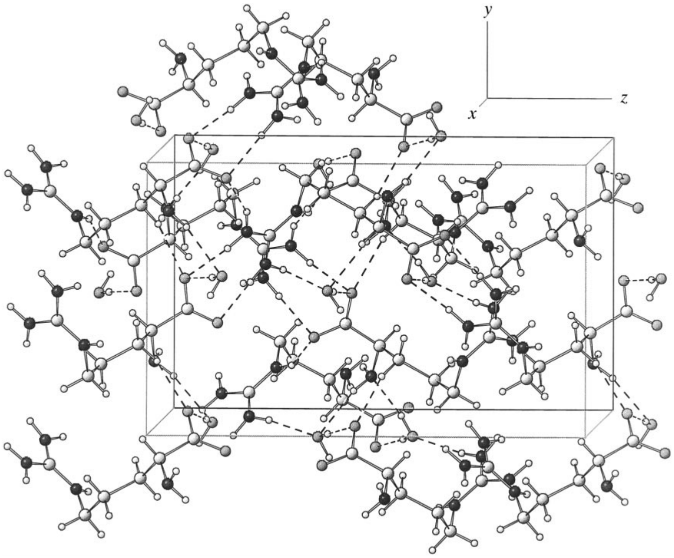


Figure 2
Packing illustration (*SCHAKAL*97; Keller, 1997) of the title compound.

This substitution of an N—H···O in lieu of an N—H···N hydrogen bond seems to have a conformational significance for the title compound. The backbone in DL-arginine monohydrate shows a less extended conformation than its close analogues cited in the discussion. The carbon chain C1–C5 is in a fully extended conformation, which holds also for the molecule in the DL-arginine dihydrate structure, but not for the L-dihydrate. However, the torsion angles (IUPAC–IUB, 1970) C3—C4—C5—N2 [χ^3 = 59.0 (1)°] and C4—C5—N2—C6 [χ^4 = 72.8 (1)°] on the other hand describe a more bent conformation in the nitrogen-rich region. This results in a near *gauche–gauche* conformation. This is different from the *trans–trans* and *trans*-perpendicular conformation observed for the L-arginine dihydrate and DL-arginine dihydrate. The underlying factor for this less extended backbone conformation in the title compound might be the N2—H10···O1$^{\rm ii}$ hydrogen bond shown by the title compound.

Experimental

Crystals of (I) were grown by slow diffusion of ethanol into a saturated aqueous solution of the amino acid. This yielded crystals suitable for the collection of a low-temperature data set.

Crystal data

$C_6H_{14}N_4O_2 \cdot H_2O$
$M_r = 192.23$
Orthorhombic, *Pbca*
$a = 11.470$ (3) Å
$b = 9.966$ (6) Å
$c = 16.023$ (1) Å
$V = 1832$ (1) Å^3
$Z = 8$
$D_x = 1.394$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15 774 reflections
$\theta = 2.54$–26.36°
$\mu = 0.111$ mm^{-1}
$T = 100$ (2) K
Plate, colourless
0.60 × 0.50 × 0.20 mm

Data collection

Nonius KappaCCD area-detector diffractometer
ω and φ scans
Absorption correction: empirical (*SORTAV*; Blessing, 1995)
$T_{\rm min} = 0.936$, $T_{\rm max} = 0.978$
41 487 measured reflections
1870 independent reflections
1862 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\rm max} = 26.36°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.080$
$S = 1.121$
1870 reflections
172 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 1.2913P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.2666 (14)	N4—C6	1.3339 (15)
O2—C1	1.2622 (15)	C1—C2	1.5427 (16)
N1—C2	1.4683 (16)	C2—C3	1.5369 (16)
N2—C6	1.3333 (15)	C3—C4	1.5305 (16)
N2—C5	1.4672 (16)	C4—C5	1.5331 (16)
C6—N2—C5	123.90 (10)	C4—C3—C2	114.06 (10)
O2—C1—O1	124.37 (11)	C3—C4—C5	112.34 (10)
O2—C1—C2	116.21 (10)	N2—C5—C4	113.37 (10)
O1—C1—C2	119.40 (10)	N2—C6—N4	121.53 (11)
N1—C2—C3	111.05 (10)	N2—C6—N3	119.54 (11)
N1—C2—C1	114.09 (10)	N4—C6—N3	118.94 (11)
C3—C2—C1	107.52 (9)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···O1*W*$^{\rm i}$	0.92 (2)	2.31 (2)	3.216 (2)	167 (2)
N2—H10···O1$^{\rm ii}$	0.87 (2)	2.02 (2)	2.828 (2)	155 (2)
N3—H71···O1$^{\rm iii}$	0.90 (2)	2.04 (2)	2.939 (2)	176 (2)
N3—H72···O1*W*$^{\rm iv}$	0.84 (2)	2.07 (2)	2.896 (2)	169 (2)
N4—H81···O2$^{\rm iii}$	0.92 (2)	1.91 (2)	2.830 (2)	174 (2)
N4—H82···O1$^{\rm v}$	0.87 (2)	2.25 (2)	3.050 (2)	152 (2)
O1*W*—H1*W*···O2	0.87 (2)	2.04 (2)	2.911 (2)	175 (2)
O1*W*—H2*W*···N1$^{\rm ii}$	0.92 (2)	1.90 (2)	2.806 (2)	169 (2)
C3—H4···O2$^{\rm i}$	1.02 (2)	2.36 (2)	3.344 (2)	164 (1)

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

Table 3
Selected torsion angles (°) of DL-arginine monohydrate, L-arginine dihydrate and DL-arginine dihydrate.

		DL-Arg monohydrate	L-Arg dihydrate	DL-Arg dihydrate
O2—C1—C2—N1		166.33 (10)		
O1—C1—C2—N1	φ^1	−15.37 (15)	−13.0 (2)	−11.5 (3)
O2—C1—C2—C3		−70.05 (13)		
O1—C1—C2—C3		108.25 (12)		
N1—C2—C3—C4	χ^1	−58.47 (13)	63.9 (2)	−54.1 (3)
C1—C2—C3—C4		176.08 (10)		
C2—C3—C4—C5	χ^2	−178.02 (10)	150.5 (2)	−179.8 (2)
C6—N2—C5—C4	χ^4	72.81 (14)	163.2 (2)	−92.2 (3)
C3—C4—C5—N2	χ^3	59.02 (13)	175.1 (2)	−163.0 (2)
C5—N2—C6—N4	χ^5	4.86 (17)	−10.1 (2)	7.4 (4)
C5—N2—C6—N3		−175.13 (10)		

All H atoms were found in the difference Fourier maps. Five types of H atoms were refined freely with a common isotropic displacement parameter for each.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996) and *SCHAKAL* (Keller, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM1417). Services for accessing these data are described at the back of the journal.

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supporting information

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Computing details

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *SCHAKAL* (Keller, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 1990).

DL-2-amino-5-guanidovaleric acid

Crystal data

$C_6H_{14}N_4O_2{\cdot}H_2O$
$M_r = 192.23$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.470$ (3) Å
$b = 9.966$ (6) Å
$c = 16.023$ (1) Å
$V = 1832$ (1) Å^3
$Z = 8$
$F(000) = 832$

$D_x = 1.394$ Mg m^{-3}
Melting point: 230 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15774 reflections
$\theta = 2.5$–26.4°
$\mu = 0.11$ mm^{-1}
$T = 100$ K
Plate, colourless
0.60 × 0.50 × 0.20 mm

Data collection

Nonius kappaCCD area detector diffractometer
Radiation source: rotating anode
Graphite monochromator
ω and φ scans
Absorption correction: empirical (using intensity measurements) (*SORTAV*; Blessing, 1995)
$T_{min} = 0.936$, $T_{max} = 0.978$

41487 measured reflections
1870 independent reflections
1862 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.5°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.080$
$S = 1.12$
1870 reflections
172 parameters
0 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 1.2913P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Experimental. An Oxford Cryosystems low temperature device was used. Reciprocal space was explored by ω and φ-scans. No intensity decay was observed. All non-hydrogen atoms were refined anisotropically.

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.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.09635 (7)	0.64767 (8)	0.62401 (5)	0.0146 (2)
O2	0.18322 (8)	0.49433 (8)	0.54327 (5)	0.0169 (2)
N1	0.00031 (9)	0.77965 (11)	0.48646 (6)	0.0164 (2)
H2	0.0240 (15)	0.8350 (17)	0.5293 (11)	0.026 (3)*
H3	−0.0658 (15)	0.7393 (18)	0.5006 (11)	0.026 (3)*
N2	0.38611 (8)	0.76189 (10)	0.30292 (6)	0.0126 (2)
H10	0.4497 (14)	0.7655 (16)	0.3321 (10)	0.022 (4)*
N3	0.46176 (9)	0.57487 (10)	0.23697 (7)	0.0143 (2)
H71	0.4476 (14)	0.5069 (16)	0.2017 (10)	0.023 (2)*
H72	0.5031 (15)	0.5588 (16)	0.2792 (10)	0.023 (2)*
N4	0.29681 (9)	0.67581 (11)	0.18398 (6)	0.0149 (2)
H81	0.3010 (14)	0.6160 (17)	0.1403 (10)	0.023 (2)*
H82	0.2491 (14)	0.7433 (17)	0.1808 (10)	0.023 (2)*
C1	0.12472 (9)	0.60032 (12)	0.55352 (7)	0.0117 (2)
C2	0.09004 (10)	0.67665 (12)	0.47352 (7)	0.0132 (2)
H1	0.0572 (12)	0.6089 (15)	0.4331 (9)	0.015 (3)*
C3	0.20162 (10)	0.73814 (12)	0.43668 (7)	0.0132 (2)
H4	0.2333 (13)	0.8049 (15)	0.4789 (9)	0.0171 (15)*
H5	0.2587 (13)	0.6624 (15)	0.4304 (9)	0.0171 (15)*
C4	0.18335 (10)	0.80988 (12)	0.35324 (8)	0.0151 (3)
H6	0.1299 (13)	0.8854 (16)	0.3610 (9)	0.0171 (15)*
H7	0.1454 (13)	0.7508 (16)	0.3150 (9)	0.0171 (15)*
C5	0.29742 (10)	0.86543 (12)	0.31729 (7)	0.0140 (2)
H8	0.2832 (12)	0.9146 (15)	0.2655 (9)	0.0171 (15)*
H9	0.3331 (13)	0.9287 (15)	0.3577 (9)	0.0171 (15)*
C6	0.38086 (10)	0.67190 (11)	0.24145 (7)	0.0115 (2)
O1W	0.41679 (8)	0.51029 (10)	0.61367 (6)	0.0209 (2)
H1W	0.3454 (19)	0.506 (2)	0.5954 (12)	0.046 (4)*
H2W	0.4469 (17)	0.584 (2)	0.5869 (12)	0.046 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0160 (4)	0.0147 (4)	0.0129 (4)	0.0021 (3)	0.0019 (3)	0.0005 (3)
O2	0.0199 (4)	0.0149 (4)	0.0158 (4)	0.0056 (3)	0.0025 (3)	0.0014 (3)
N1	0.0129 (5)	0.0199 (6)	0.0165 (5)	0.0043 (4)	0.0025 (4)	0.0043 (4)
N2	0.0099 (5)	0.0154 (5)	0.0126 (5)	−0.0012 (4)	−0.0010 (4)	−0.0020 (4)
N3	0.0154 (5)	0.0149 (5)	0.0125 (5)	0.0014 (4)	−0.0019 (4)	−0.0004 (4)
N4	0.0159 (5)	0.0144 (5)	0.0145 (5)	0.0022 (4)	−0.0034 (4)	−0.0024 (4)
C1	0.0087 (5)	0.0130 (5)	0.0134 (5)	−0.0015 (4)	0.0009 (4)	0.0014 (4)
C2	0.0124 (5)	0.0148 (6)	0.0123 (5)	0.0010 (5)	0.0004 (4)	0.0003 (4)
C3	0.0118 (5)	0.0144 (5)	0.0135 (6)	0.0004 (5)	0.0005 (4)	0.0007 (5)
C4	0.0129 (6)	0.0174 (6)	0.0149 (6)	0.0018 (5)	0.0015 (5)	0.0028 (5)
C5	0.0159 (6)	0.0123 (5)	0.0140 (6)	−0.0001 (4)	0.0020 (5)	0.0000 (5)
C6	0.0107 (5)	0.0126 (5)	0.0111 (5)	−0.0039 (4)	0.0025 (4)	0.0023 (4)
O1W	0.0179 (5)	0.0225 (5)	0.0223 (5)	−0.0050 (4)	−0.0035 (4)	0.0087 (4)

Geometric parameters (Å, º)

O1—C1	1.2666 (14)	C1—C2	1.5427 (16)
O2—C1	1.2622 (15)	C2—C3	1.5369 (16)
N1—C2	1.4683 (16)	C2—H1	1.009 (15)
N1—H2	0.922 (18)	C3—C4	1.5305 (16)
N1—H3	0.888 (18)	C3—H4	1.016 (15)
N2—C6	1.3333 (15)	C3—H5	1.005 (15)
N2—C5	1.4672 (16)	C4—C5	1.5331 (16)
N2—H10	0.867 (16)	C4—H6	0.978 (15)
N3—C6	1.3422 (16)	C4—H7	0.955 (16)
N3—H71	0.898 (17)	C5—H8	0.977 (15)
N3—H72	0.842 (17)	C5—H9	0.992 (15)
N4—C6	1.3339 (15)	O1W—H1W	0.87 (2)
N4—H81	0.920 (17)	O1W—H2W	0.92 (2)
N4—H82	0.868 (17)		
C2—N1—H2	108.5 (10)	C4—C3—H4	109.0 (8)
C2—N1—H3	108.6 (11)	C2—C3—H4	107.7 (8)
H2—N1—H3	109.4 (15)	C4—C3—H5	110.7 (8)
C6—N2—C5	123.90 (10)	C2—C3—H5	106.4 (8)
C6—N2—H10	117.7 (11)	H4—C3—H5	108.9 (11)
C5—N2—H10	118.0 (11)	C3—C4—C5	112.34 (10)
C6—N3—H71	116.9 (10)	C3—C4—H6	109.5 (9)
C6—N3—H72	118.9 (11)	C5—C4—H6	107.7 (9)
H71—N3—H72	117.7 (15)	C3—C4—H7	109.6 (9)
C6—N4—H81	117.9 (10)	C5—C4—H7	111.8 (9)
C6—N4—H82	121.2 (10)	H6—C4—H7	105.6 (12)
H81—N4—H82	119.4 (14)	N2—C5—C4	113.37 (10)
O2—C1—O1	124.37 (11)	N2—C5—H8	109.6 (8)
O2—C1—C2	116.21 (10)	C4—C5—H8	111.0 (8)

O1—C1—C2	119.40 (10)	N2—C5—H9	105.3 (9)
N1—C2—C3	111.05 (10)	C4—C5—H9	109.6 (9)
N1—C2—C1	114.09 (10)	H8—C5—H9	107.7 (12)
C3—C2—C1	107.52 (9)	N2—C6—N4	121.53 (11)
N1—C2—H1	107.3 (8)	N2—C6—N3	119.54 (11)
C3—C2—H1	109.3 (8)	N4—C6—N3	118.94 (11)
C1—C2—H1	107.5 (8)	H1W—O1W—H2W	103.6 (17)
C4—C3—C2	114.06 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···O1*W*$^{\text{i}}$	0.92 (2)	2.31 (2)	3.216 (2)	167 (2)
N2—H10···O1$^{\text{ii}}$	0.87 (2)	2.02 (2)	2.828 (2)	155 (2)
N3—H71···O1$^{\text{iii}}$	0.90 (2)	2.04 (2)	2.939 (2)	176 (2)
N3—H72···O1*W*$^{\text{iv}}$	0.84 (2)	2.07 (2)	2.896 (2)	169 (2)
N4—H81···O2$^{\text{iii}}$	0.92 (2)	1.91 (2)	2.830 (2)	174 (2)
N4—H82···O1$^{\text{v}}$	0.87 (2)	2.25 (2)	3.050 (2)	152 (2)
O1*W*—H1*W*···O2	0.87 (2)	2.04 (2)	2.911 (2)	175 (2)
O1*W*—H2*W*···N1$^{\text{ii}}$	0.92 (2)	1.90 (2)	2.806 (2)	169 (2)
C3—H4···O2$^{\text{i}}$	1.02 (2)	2.36 (2)	3.344 (2)	164 (1)

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