Fig. 2. View of crystal packing along a.

(Ramakrishnan, Seshadri & Viswamitra, 1984). Fig. 2 shows that the tyrosyl rings do not stack in the crystal lattice. The lone water molecule forms hydrogen bonds with the amino and carboxyl terminal atoms of the dipeptide molecules (Table 2d).

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Structure of L-Arginyl-L-aspartic Acid Dihydrate

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Abstract. $C_{10}H_{19}N_5O_5.2H_2O$, $M_r = 325.32$, monoclinic, $P2_1$, $a = 12.029$ (2), $b = 4.904$ (2), $c = 13.215$ (2) Å, $\beta = 107.68$ (2)°, $V = 743$ (1) Å^3, $Z = 2$, $D_m = 1.45$, $D_x = 1.45$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1.54184$ Å, $\mu = 1.01$ mm^{-1}, $F(000) = 348$, $T = 293$ K. The final R value for 1277 observed reflections $[I_o \geq 3\sigma(I_o)]$ is 0.031. The dipeptide exists as a zwitterion. The arginyl side-chain conformation is similar to that found in arginyl-glutamic acid [Pandit, Seshadri & Viswamitra (1983). *Acta Cryst.* C39, 1669–1672]. The guanidyl group forms a pair of hydrogen bonds with oxygen atoms of the backbone carboxyl group. The crystal structure is also stabilized by H-bonding interactions involving both water molecules.

Introduction. The arginine side chain is expected to play an important role in the specific recognition process between proteins and nucleic acids. In view of this interest we have initiated a study of arginine-containing peptides (Pandit, Seshadri & Viswamitra, 1983) and their complexes with nucleotides. We report here the crystal structure of L-arginyl-L-aspartic acid as part of this study.

Experimental. The dipeptide was purchased from Sigma Chemicals and used without further purification. Thin needle crystals of the peptide alone appeared in our attempts to complex it with oligonucleotides, using 2-methyl-2,4-pentanediol (MPD) vapour-diffusion methods. The size of the crystal used for X-ray data collection was $0.05 \times 0.1 \times 0.5$ mm. The cell parameters were initially determined from Weissenberg photographs and were later refined on a CAD-4 diffractometer using 25 high-angle ($10 \leq \theta \leq 51°$) reflections. Three-dimensional intensity data were collected up to $\theta = 70°$ using ω–2θ scans. Three standard reflections during the data collection showed no significant variation in their intensities, indicating that the crystal was stable to X-rays. The range of indices was $h = 0$ to 14, $k = 0$ to 5 and $l = -15$ to 14. A total of 1277 reflections was considered observed $|I \geq 3\sigma(I)|$ out of 1587 collected. Lorentz and polarization corrections were applied but no absorption correction was made.

The structure was solved using *MULTAN*11/82 (Germain, Main & Woolfson, 1971). Non-hydrogen atoms were refined anisotropically using full-matrix methods. All hydrogen atoms were located from difference Fourier maps and refined isotropically. The final $R = 0.031$ and $wR = 0.029$, where the weight w is $1/|\sigma(F_o)|^2$. The function minimized was $\sum w(|F_o| - |F_c|)^2$. The average $\Delta/\sigma = 0.02$; $\Delta\rho$ variations in the

Table 1. *Positional parameters and their estimated standard deviations*

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

|	x	y	z	$B_{eq}(\text{Å}^2)$
O1	0·9982 (2)	0·613	0·4076 (2)	2·06 (5)
O2	0·6620 (2)	0·4778 (6)	0·0949 (2)	2·69 (5)
O3	0·8484 (2)	0·3608 (6)	0·1542 (2)	2·27 (5)
O4	0·7531 (2)	1·0088 (6)	0·4293 (2)	3·07 (6)
O5	0·6065 (2)	1·2471 (6)	0·3232 (2)	2·51 (5)
OW1	1·0043 (2)	0·4469 (7)	0·0501 (2)	3·59 (6)
OW2	0·5703 (3)	0·437 (1)	0·5056 (2)	6·04 (9)
N1	1·1551 (2)	1·0116 (7)	0·4684 (2)	2·31 (6)
N2	0·8837 (2)	0·8578 (6)	0·2700 (2)	1·75 (5)
N3	1·3812 (2)	1·2628 (7)	0·1726 (2)	2·16 (6)
N4	1·4269 (2)	1·5839 (7)	0·0642 (2)	2·23 (6)
N5	1·2367 (2)	1·4609 (8)	0·0342 (2)	2·27 (6)
C1	1·0805 (2)	1·0148 (7)	0·3546 (2)	1·51 (6)
C2	0·9824 (2)	0·8102 (7)	0·3467 (2)	1·49 (6)
C3	0·7789 (2)	0·6920 (7)	0·2548 (2)	1·59 (6)
C4	0·7606 (2)	0·4989 (8)	0·1590 (2)	1·76 (6)
C5	1·1522 (2)	0·9349 (8)	0·2817 (2)	2·09 (7)
C6	1·2337 (3)	1·1635 (8)	0·2676 (3)	2·03 (7)
C7	1·3042 (3)	1·0594 (8)	0·1964 (3)	2·33 (7)
C8	1·3484 (2)	1·4334 (8)	0·0909 (2)	1·81 (6)
C9	0·6723 (2)	0·8681 (8)	0·2470 (2)	1·83 (6)
C10	0·6789 (3)	1·0557 (8)	0·3407 (2)	1·84 (7)
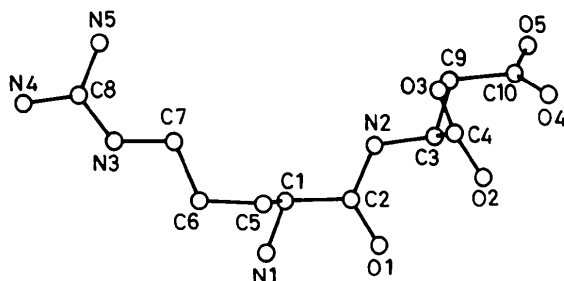
Fig. 1. Molecular structure and atomic numbering.

final difference Fourier map were within ± 0.13 e Å^{-3}. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All computations were performed on a PDP 11/44 computer using the structure determination package supplied by Enraf–Nonius (1979).

Discussion. The final positional and thermal parameters are given in Table 1* and molecular geometry is listed in Table 2. The molecular structure and atomic numbering scheme are shown in Fig. 1. The dipeptide exists as a zwitterion with the terminal N atom protonated. The peptide bond is planar with the

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51177 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Molecular geometry of* L-*arginyl-*L-*aspartic acid*

Numbers in parentheses are estimated standard deviations in the least significant digits.

(*a*) Bond distances (Å)

O1–C2	1·237 (3)	N4–C8	1·328 (5)
O2–C4	1·235 (4)	N5–C8	1·333 (3)
O3–C4	1·272 (5)	C1–C2	1·527 (4)
O4–C10	1·260 (3)	C1–C5	1·527 (5)
O5–C10	1·254 (4)	C3–C4	1·543 (5)
N1–C1	1·500 (3)	C3–C9	1·523 (5)
N2–C2	1·327 (3)	C5–C6	1·537 (5)
N2–C3	1·462 (5)	C6–C7	1·533 (5)
N3–C7	1·460 (5)	C9–C10	1·525 (5)
N3–C8	1·328 (4)		

(*b*) Bond angles (°)

C2–N2–C3	122·9 (3)	O2–C4–O3	124·1 (3)
C7–N3–C8	123·7 (2)	O2–C4–C3	118·8 (3)
N1–C1–C2	106·1 (3)	O3–C4–C3	117·0 (2)
N1–C1–C5	110·5 (2)	C1–C5–C6	113·1 (4)
C2–C1–C5	111·2 (3)	C5–C6–C7	108·8 (3)
O1–C2–N2	124·0 (3)	N3–C7–C6	114·2 (3)
O1–C2–C1	120·5 (2)	N3–C8–N4	120·5 (2)
N2–C2–C1	115·4 (3)	N3–C8–N5	121·4 (3)
N2–C3–C9	111·5 (3)	C3–C9–C10	116·8 (2)
C4–C3–C9	112·7 (2)		

(*c*) Torsion angles (in °, average e.s.d. 0·3°)

N1–C1–C2–N2	ψ_1	153·1
C2–N2–C3–C4	φ_2	−104·6
C1–C2–N2–C3	ω	−176·4
N1–C2–C5–C6	χ^1	−75·4
C1–C5–C6–C7	χ^2	−178·1
C5–C6–C7–N3	χ^3	177·1
C6–C7–N3–C8	χ^4	−88·3
C7–N3–C8–N5	χ^{51}	11·1
C7–N3–C8–N4	χ^{52}	−169·6
N2–C3–C9–C10	χ^1	−57·8
C3–C9–C10–O4	χ^{21}	−19·3
C3–C9–C10–O5	χ^{22}	169·2

(*d*) Hydrogen-bond distances and angles; average e.s.d.'s in distances 0·01 Å and in angles 5°

A–H$\cdots B$	$A\cdots B$ (Å)	A–H$\cdots B$ (°)	Unit-cell translation of atom B	Symmetry code
N1–H1$\cdots$O4	2·87	158	−2 0 −1	ii
N1–H2$\cdots$O4	2·84	120	−1 0 −1	ii
N1–H3$\cdots$O1	2·86	130	2 0 1	ii
N2–H$\cdots$O3	2·87	169	0 1 0	i
N3–H$\cdots$O5	2·84	172	1 0 0	i
N4–H1$\cdots$O2	2·82	158	1 1 0	i
N4–H2$\cdots$O2	2·78	177	−2 2 0	ii
N5–H1$\cdots$OW1	2·87	142	0 1 0	i
N5–H2$\cdots$O3	3·09	173	−2 −2 0	ii
OW1–H1$\cdots$O3	2·68	170	0 0 0	i
OW1–H2$\cdots$OW1	2·77	164	2 0 0	ii
OW2–H1$\cdots$OW2	2·96	128	−1 1 −1	ii
OW2–H2$\cdots$O5	2·74	176	0 −1 0	i

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

conformational angle $\omega = -178.4$ (3)° (IUPAC–IUB Commission on Biochemical Nomenclature, 1970). The arginyl side-chain conformation (Table 2c) is similar to that found in arginyl-glutamic acid (Pandit, Seshadri & Viswamitra, 1983). The aspartic acid side-chain conformational angles χ^1, χ^{21} and χ^{22} are −57·8 (3), −19·3 (3) and 169·2 (3)°, respectively.

The N4 and N5 atoms of the guanidyl group are hydrogen bonded to the backbone carboxyl-group
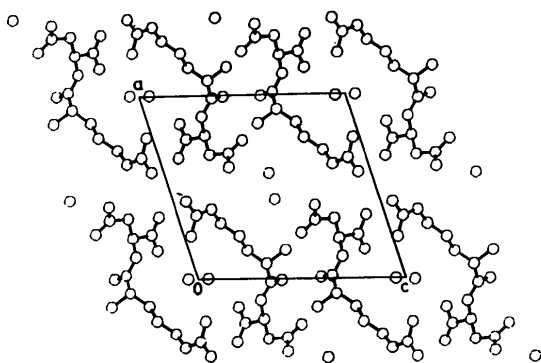
Fig. 2. View of crystal packing along **b**.

oxygen atoms O2 and O3 respectively (Table 2d). This is in contrast to the structure of arginyl-glutamic acid which shows specific H-bonding interactions between the guanidyl group and carboxyl oxygen atoms of the

glutamic acid side chain (Pandit, Seshadri & Viswamitra, 1983). Fig. 2 and Table 2(d) show that the two water molecules in the asymmetric unit form independent water chains along **b**. These chains are also H-bonded to the L-arginyl-L-aspartic acid residues.

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Conformational Aspects of *meso*-Tartaric Acid. XI.* Structure of Lithium Hydrogen *meso*-Tartrate Monohydrate

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Abstract. $Li^+.C_4H_5O_6^-.H_2O$, $M_r = 174.04$, monoclinic, $P2_1/c$, $a = 4.8848$ (2), $b = 25.366$ (2), $c = 5.3107$ (4) Å, $\beta = 95.768$ (5)°, $V = 654.71$ (7) Å^3, $Z = 4$, $D_x = 1.766$ g cm^{-3}, $\lambda(Mo\,K\alpha) = 0.71073$ Å, $\mu = 1.6$ cm^{-1}, $F(000) = 360$, $T = 294$ K, $R = 0.042$, $wR = 0.048$ for 2326 observed reflections with $I \geq 2.5\sigma(I)$. The crystal structure is a racemate of two conformational antipodes of the *meso*-tartrate anion, which has adopted its usual *gauche* conformation with respect to the carbon chain. The glycolic acid parts are almost planar. The Li$^+$ ion is irregularly coordinated to five O atoms at a mean distance of 2.05 (6) Å.

Introduction. The crystal structure determination of the title compound is part of the research program which is being carried out on the molecular conformational aspects of neutral *meso*-tartaric acid and its ionized forms. A second point of interest is the nature of hydrogen-bond schemes in acid salts in general.

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* Part X: Blankensteyn & Kroon (1986).

Experimental. Suitable crystals were obtained from an aqueous solution. An Enraf–Nonius CAD-4 diffractometer (Mo $K\alpha$ radiation, $\omega/2\theta$ scan) was used for intensity measurements. A colorless crystal $1.0 \times 0.7 \times 0.2$ mm was glued on top of a glass fiber. Accurate cell parameters were calculated from setting angles of 20 reflections (Cu $K\alpha$, $30 < \theta < 44°$) in four alternative settings. 3023 reflections were measured (h: $-7 \rightarrow 7$, k: $0 \rightarrow 40$, l: $0 \rightarrow 8$) of which 2328 with $I \geq 2.5\sigma(I)$, $0.8 < \theta < 35°$. Three reflections (200, 0,10,0, 002) were measured every 2 h and showed no systematic decrease during the experiment. A ψ-scan for the reflection 0$\bar{1}$3 showed an intensity variation up to 7.0% about the mean. Intensities were corrected for Lorentz and polarization effects, not for absorption. Variance $\sigma^2(I)$ was calculated based on counting statistics plus a term $(PI)^2$ where $P(=0.013)$ is the instability constant (McCandlish, Stout & Andrews, 1975). The structure was solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined on