Table 1. *Cell dimensions*

Peptide	Habit	Symmetry	a (Å)	b (Å)	c (Å)	β (°)	Space group	Density (g.cm.$^{-3}$)	$n_{calc.}$	Symmetry number
A	Prisms {110}, {100}	Orthorhombic	7·92	20·56	7·56	—	$P2_12_12_1$	1·510	—	4·00
B	Needles or plates on {001}	Monoclinic	6·57	5·49	16·94	98	$P2_1$	1·350	2·00	2·00
C	Plates on {001}	Monoclinic	5·44	6·48	20·36	91·5	$P2_1$	1·203	—	2·00
D	(1) Needles or plates on {010}	Orthorhombic	22·37	23·34	11·34	—	$A2_122$	1·28	7·98	8·00
	(2) Needles	Orthorhombic	18·26	28·04	11·42	—	$P22_12$	1·29	7·97	4·00

A α-L-Glutamyl aspartic acid monohydrate.
B α-L-Glutamyl-L-valine.
C α-L-Glutamyl-L-leucine.
D *p*-Brombenzoyl-L-leucyl-D-phenylalanyl-L-proline methyl ester.

presumably owing to the increased possibilities of hydrogen bonding.

p-Brombenzoyl-L-leucyl-D-phenylalanyl-L-proline methyl ester

The original sample consisted of very small orthorhombic needles and plates on (010), c the needle axis. The space group was found to be $A2_122$. The density of the crystals obtained experimentally and unit-cell dimensions are shown in Table 1. The calculated number of molecules in the unit cell is 7·98, that required by symmetry being 8·00.

Attempts were made to grow larger crystals from ethyl acetate/petrol ether mixture and from a number of other organic solvents. A second crystalline form was always obtained, consisting of rosettes of long, thin, fibrous needles. The symmetry of this form is also orthorhombic, but the space group is now $P22_12$.

The measured density is 1·29 g.cm.$^{-3}$ and the number of molecules in the unit cell computed from the figures in the table is 7·97. This is twice that required by the crystal symmetry and hence there must be two independent molecules in the asymmetric unit.

When it was first examined it was hoped that the tripeptide unit might show some form of intramolecular hydrogen bonding and thus might suggest a configuration for folded polypeptide chains. Infra-red studies, however, have shown the molecule to have an extended configuration, at least in the first crystalline form (Abbott & Ambrose, 1953).

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The accuracy of electron-density maps in X-ray analysis: correction.

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Incorrect formulae for the standard deviations of the x and z atomic coordinates in a monoclinic cell have been given by Cruickshank (1949), equation (11·14). These lead to the unlikely result that errors are larger in monoclinic than in orthorhombic cells. On assuming statistical spherical symmetry of the $|F(hkl)|$ errors in reciprocal space ($\sigma(A_h) = \sigma(A_k) = \sigma(A_l)$), and spherical symmetry of the atomic peak ($A_{hh} = A_{kk} = A_{ll}$), a revised analysis allowing for the correlation of A_h and A_l (covariance $(A_h, A_l) = \cos\beta\sigma^2(A_k)$) shows that

$$\sigma(x) = \sigma(y) = \sigma(z) = \sigma(A_k)/A_{kk}\,.$$

Reference

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