CRYSTALLOGRAPHY IN BIOCHEMISTRY AND PHARMACOLOGY

03.2-6 CYCLIC Dipeptides containing proline. The crystal structure and conformation of cyclo(-L-Phe-L-Pro-). By F. Mazza, Istituto di Strutturistica Chimica "G. Giacomello" CNR, C.P. n. 10, 00016 Monterotondo Stazione, Roma and by F. Pinnen, G. Zanotti and G. Lucente, Istituto di Chimica Farmaceutica, Facoltà di Farmacia, Università di Roma "La Sapienza", 00185 Roma (Italy).

Cyclic oligopeptides, both in the solid state and in solution, represent important and valuable models to gain information on peptides and proteins. A large number of data have been obtained by studying cyclic systems containing amino acids with aromatic side-chains and/or cyclic imino acids. The constraint imposed by the presence of an additional ring and the possible interaction between the aromatic side chain with the peptide bonds have focused the attention on these models. As continuation of our studies in this field (S. Cerrini, W. Fedeli, G. Lucente, F. Mazza, F. Pinnen and G. Zanotti, Int. J. Peptide Protein Res., 1983,22) we here report the crystal and molecular structure of cyclo(-L-Phe-L-Pro-):C/H/N/O; clinico, s.g.P2₁̅; α=10.789(2), b=10.061(2), c=6.668(3) Å, β=92.70(3)°, V=614.5(5) Å³, Z=2.

The structure has been solved by MULTAN and refined to a final R and R₁, respectively of 0.038 and 0.054 for 1985 independent reflections with ID-2.04(1). The conformation of the molecule is shown in the Figure.

03.2-7 Observation of a highly extended parallel chain z-piloted sheet arrangement: The crystal structure of L-valyl-glycyl-glycine. By V.Lalitha, B.Murali and E.Subramanian, Department of Crystallography and Biophysics, University of Madras, Madras-600 025, India.

The tripeptide, L-valyl-glycyl-glycine, crystallizes from water in the monoclinic space group C₂ with a=24.056(3), b=4.400(1), c=10.623(2) Å, β=110.02(1)°, Z=4. OMe integrity data for 815 reflections (sinθ/λ<0.53 Å⁻¹) from a diffractometer were used to solve the structure by direct methods using SHELXS4 computer program and to refine the structure anisotropically to a final R-index of 0.045.

The peptide chain has an extended all trans conformation, with θ₁=123.1°, θ₂=-173.5°, θ₃=-155.1°, η₁=154.7°, η₂=170.7°, η₃=-146.6°, and η₄=180.0°. The peptide chain repeat distance (10° = 30°) is 7.25 Å. The conformation of the valyl side chain is given by 

\[ \gamma = -52.5°, \gamma = -174.2° \]

Two interpeptide hydrogen bonds (3.05 Å, 3.05 Å) between adjacent molecules related by the translation of the lattice give rise to the familiar extended parallel chain pleated β-sheet arrangement, with angles at hydrogen atoms of 143° and 151°. The conformation adopted by the molecule in forming the parallel chain arrangement appears to be the most extended in comparison to all previous observations.