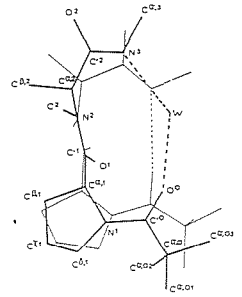
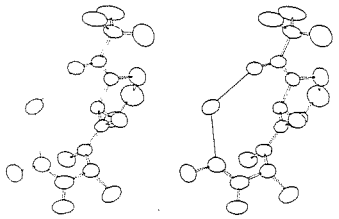
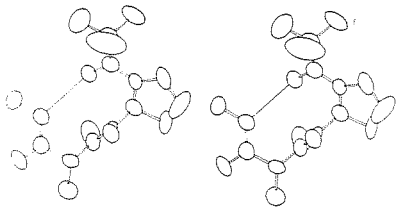


Projection des deux molécules sur les squelettes peptidiques



Vues stéréoscopiques des molécules



03.2-09 X-RAY STUDIES OF AMINO ACID - VITAMIN INTERACTIONS. THE CRYSTAL STRUCTURE OF LYSINE PANTOTHENATE. By D.M. Salunke and M. Vijayan, Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012, India.

Non-covalent interactions play a crucial role in the structure, binding and action of proteins. As part of an attempt to study, at the atomic resolution, the possible geometrical features of such interactions through the x-ray analysis of crystalline complexes of amino acids and short peptides among themselves as well as with other biomolecules (Acta Cryst. (1980) B36, 125-128, and the references therein), the crystal structure of a 1:1 complex between lysine and pantothenic acid has been determined. The complex crystallizes in the monoclinic space group $P2_1$ with two formula units in a cell of dimensions a = 5.883, b = 16.218, c = 10.024 Å and β = 106.6°. The structure, solved by the direct method, has been refined to a current R value of 0.059 for 1868 observed reflections. The zwitterionic positively charged lysine molecules in the structure exist in the fully extended conformation whereas the pantothenate anions have a somewhat folded structure. The unlike molecules aggregate into separate alternating layers in the crystal structure as in several other crystalline complexes involving amino acids. Among the interactions which hold the adjacent layers together, those involving the side chain amino group of lysine and the carboxylate group in the pantothenate anion are of particular interest.

03.2-10 CRYSTAL STRUCTURES OF 4-NITRO-L-HISTIDINE AND $N^{(\alpha)}$-ACETYL-4-NITRO-L-HISTIDINE. By X. Solans, and M. Font-Altaba. Dept. Crystallography and Mineralogy, University of Barcelona, Gran Via 585, Barcelona-7. Spain.

4-Nitro-L-histidine, monohydrate (I): $C_6H_8N_4O_4 \cdot H_2O$, orthorhombic, $P2_12_12_1$, Z = 4, a = 12.519 (4), b = 10.757(3), c = 6.590(1) Å, V = 887.5 (7) $Å^3$, Dc = 1.63 Mg m^{-3}. 1127 observed reflections.

$N^{(\alpha)}$-acetyl-4-nitro-L-histidine (II): $C_8H_{10}N_4O_5$ orthorhombic, $P2_12_12_1$, Z = 4, a = 15.425(3), b = 9.756(2), c = 6.822(1) Å, V = 1026.6(7) $Å^3$, Dc = 1.57 Mg m^{-3}. 1534 observed reflections

Intensity data were recorded on a Philips PW-1100 four-circle diffractometer, and both structures were solved using MULTAN80 system of computer programs and refined by full-matrix least-squares method using SHELX76 program. The final R values are 0.045 for (I) and 0.063 for (II).

The nitro substituent modifies the bond distances in the imidazolyl ring with respect to those obtained in the L-histidine. The torsion angles are similar to those obtained in the L-histidine, with the exception of -C-COOH bond in the $N^{(\alpha)}$-acetyl-4-nitro-L-histidine, which is twisted -98.5?

The packing of the molecules is due in the two compounds to hydrogen bonds, which are different in each structure.