

Two pentadehydropeptides with different configurations of the Δ Phe residues.

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Streszczenie

Comparison of the crystal structures of two pentadehydropeptides containing Δ Phe residues, namely (Z,Z)-N-(tert-butoxycarbonyl)glycyl- α,β -phenylalanylglycyl- α,β -phenylalanylglycine (or $\text{Boc}^0\text{-Gly}^1\text{-}\Delta^Z\text{Phe}^2\text{-Gly}^3\text{-}\Delta^Z\text{Phe}^4\text{-Gly}^5\text{-OH}$) methanol solvate, $\text{C}_{29}\text{H}_{33}\text{N}_5\text{O}_8\cdot\text{CH}_4\text{O}$, (I), and (E,E)-N-(tert-butoxycarbonyl)glycyl- α,β -phenylalanylglycyl- α,β -phenylalanylglycine (or $\text{Boc}^0\text{-Gly}^1\text{-}\Delta^E\text{Phe}^2\text{-Gly}^3\text{-}\Delta^E\text{Phe}^4\text{-Gly}^5\text{-OH}$), $\text{C}_{29}\text{H}_{33}\text{N}_5\text{O}_8$, (II), indicates that the $\Delta^Z\text{Phe}$ residue is a more effective inducer of folded structures than the $\Delta^E\text{Phe}$ residue. The values of the torsion angles ϕ and ψ show the presence of two type-III' β -turns at the $\Delta^Z\text{Phe}$ residues and one type-II β -turn at the $\Delta^E\text{Phe}$ residue. All amino acids are linked *trans* to each other in both peptides. β -Turns present in the peptides are stabilized by intramolecular 4 $\rightarrow$ 1 hydrogen bonds. Molecules in both structures form two-dimensional hydrogen-bond networks parallel to the (100) plane.

Adres publiczny

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