

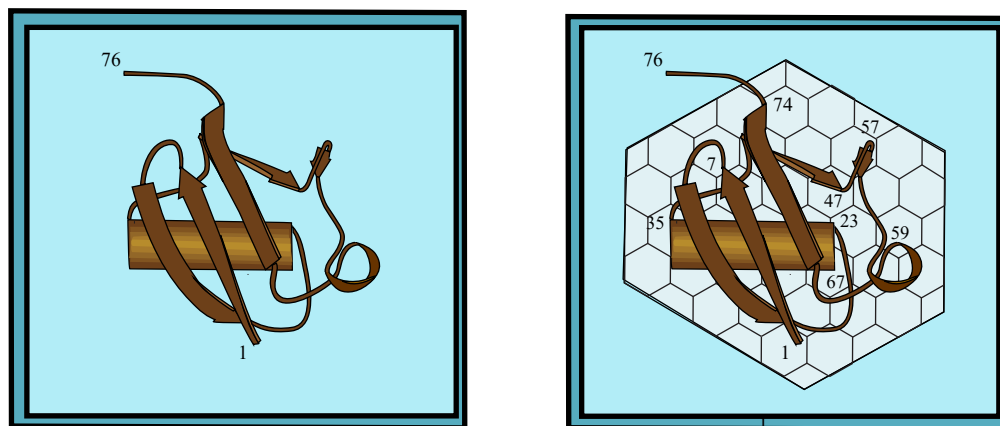


CUBIC HYDRATION OF UBIQUITIN AND ITS POLYPEPTIDE

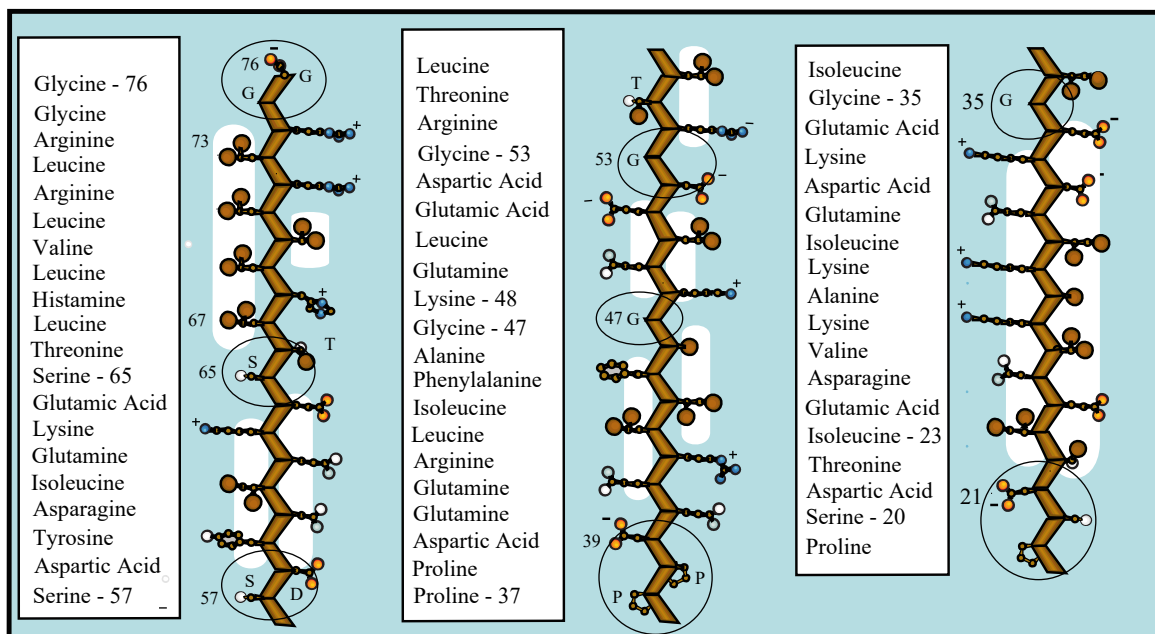
J. C. Collins, PhD

Dedicated to the late Professors Carl Djerassi and William S. Johnson of Stanford University.

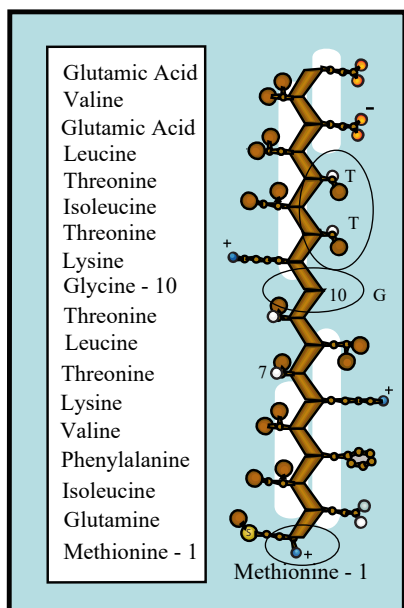
Ubiquitins are a family of proteins which are present in almost every living cell. By attaching the 76 glycine ends of their flexible tails to damaged proteins, they take them to enzymes where they are degraded back to aminoacids. Ubiquitins are so prevalent that they are considered to be fundamental cleaning proteins of life.¹



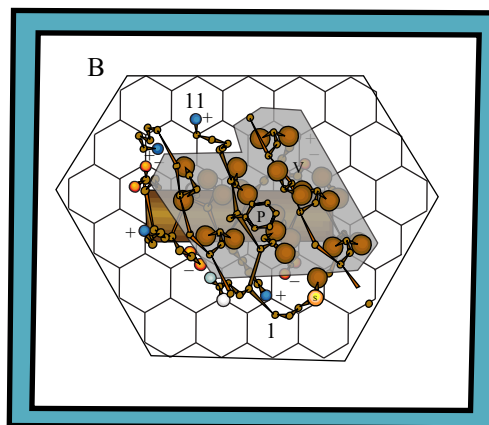
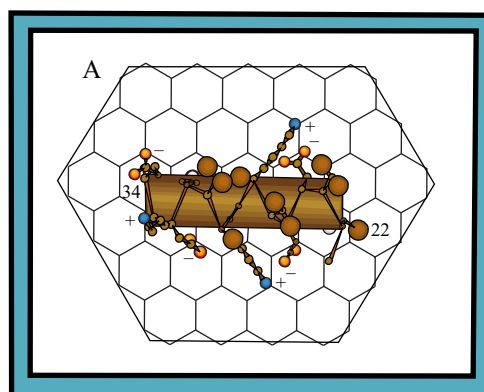
When viewed as shown above,² the coil and linear segments tend to follow the basic cubic patterning of the cubic lattice of water molecules (2.76 Angstroms apart as they are in cubic ice).³



Regions of the polypeptide which do not hydrogen-bond with surface water induce the formation of adjacent transient linear elements of hydration are shown above with a white background, while regions which bond with surface water are circled. Between glycine 35 to aspartate 21, water, by forming linear elements on both sides of the polypeptide, introduces so much instability that the segment that it rotates into the lower-energy coil.⁴ A second small coil between serine 65 and serine 57 forms perpendicular to the plane. As you can see, all three segments in the beta-sheet tend to follow hydration patterning.



The first nine peptides in the chain, as shown on the left, shield the chain from hydration, but fit so well into the front-side of the coil that they remain as a linear segment and follow surface hydration.



The ubiquitin structure is unique in having an exceptionally large number of cationic lysine peptides. Even the coil, as in A, has two that extend out in the plane with their terminal amines in matrix positions of water molecules. The positive charge on the molecule, draws the negative ends of polypeptides in to the glycine-glycine 47 end to be towed to a lytic enzyme for cleavage back to aminoacids.

The upper surface of the coil is highly lipophylic with two isoleucines and a valine providing a flat upper face to induce the formation of covalent linear elements on an upper level. As shown in B, an isoleucine and valine extend down toward the coil while a phenylalanine (P) and valine (V) provide a lipid upper surface for binding aeromatic and lipid regions of guest polypeptides. The continuing polypeptide passes out of the cubically-patterned region through two lysines to the two glycines on the end.¹

It is amazing that prolines, threonines, glycines and serines, are in specific positions in the chains of natural polypeptides such as this, to permit lipid regions to form such firm complimentary unions that all water between them is released. When the earliest phases of random polypeptide synthesis began, it appears that it was sequences of aminoacids which could spontaneously bring their lipid surfaces together to form tight unions release all surface water between them, survived. Those that could not release the water were destabilized by its dynamics and carried to lytic enzymes by ubiquitins.

References

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