

*Probing effect of packing motif on helical assembly*

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Oligomerization of  $\alpha$ -helices is principle to a myriad of biological functions such as ion transporter, cell surface receptors, transcription factors etc. The interactions between the  $\alpha$ -helices are mediated by signature structural motifs at the interface of the helices. It is typically made up by small amino acids as glycine (could be serine or alanine as well) placed at  $i$  and  $i+4$  positions at the helix-helix interface giving rise to the GXXXG motif [Kleiger et al. 2002, Senes et al. 2004]. De novo design of proteins from the first principles have let to the creation of a plethora of designed proteins with sequence directed functions, having wide range of applications as molecular scaffolds, nanoparticle templates, biomaterials. One such designed protein id P6 protein by Lanci et al. 2012, where incorporation of the GXXXG motif in the sequence imparts it with the desirable property of self-assembly. P6-a with the motif GXXXG in the centre of the helix and which leads to the oligomerization as trimers in parallel fashion. Six such trimeric units come together to form a hexameric honeycomb like structure, where these trimers are arranged in anti-parallel. When this motif is shifted one turn down the helix (P6-d), the parallel trimeric units now assemble in parallel to form the honeycomb structure. We are interested to find out if changing the GXXXG motif to different structural motifs: SXXXS / AXXXXA / GXXXXA will affect the self-assembly of this molecule. To this end we have synthesised four peptides P6-a1 with SXXXS motif, P6-a2 with AXXXXA motif, P6-d1 with SXXXS motif and P6-d3 with GXXXXA motif. We crystallized P6-a1, P6-a2, P6-d1 and P6-d3. Diffraction data has been collected at Home Source and structures have been solved using molecular replacement. We anticipate our results will be pivotal in understanding packaging motif driven self-assembly of molecules and contribute to the field of protein designing.

1. Kleiger et al. (2002), *Biochemistry*, 41, 5990-5997
2. Senes et al. (2004), *Current Opinion in Structural Biology*, 14, 465-479
3. Lanci et al. (2012), *PNAS*, 109, 7304-7309

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