

What is the purpose of using multiple seeds and recycling cycles in AlphaFold predictions? Explain the difference between seeds and recycles.

AF uses stochastic sampling and iterative refinement to explore conformational space. A recycle is a single pass of feeding the predicted structure back into the network so that AF can refine it. After the initial backbone production, the structure and internal representations are fed back into the Evoformer, gradually improving coord., distance predictions and attention maps. Aim is to improve accuracy by gradually refining the structure. Seeds provide the initial randomness. Changing the seed creates a different conformational pathway, often yielding to different structures. Using multiple seeds allows us to include randomness in the predictions thus to sample alternative conformations. In other words, it helps escaping the local minima.