

RamaRota

ϕ , ψ , χ^1 analysis

June 2026

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- There is a clear χ^1 dependence for all side-chain types
 - ...as measured by the MMD² of the χ^1 clusters
 - (Orange and Red blocks in the heat map)
- AlphaFold2 models have generally more dramatic differences
 - ...probably due to tighter distributions
- AlphaFold2 models typically recapitulate the χ^1 distributions (although somewhat tighter)
 - ...but some do not (*e.g.* GLN, GLU, MET)

AlphaFold2 sampling

- Steinegger: steineggerlab foldseek
- Nature 2023, "Clustering predicted structures at the scale of the known protein universe" Barrio-Hernandez **622**, pages 637–645 (2023)
- Then the representative structures were downloaded from the AlphaFold DB.