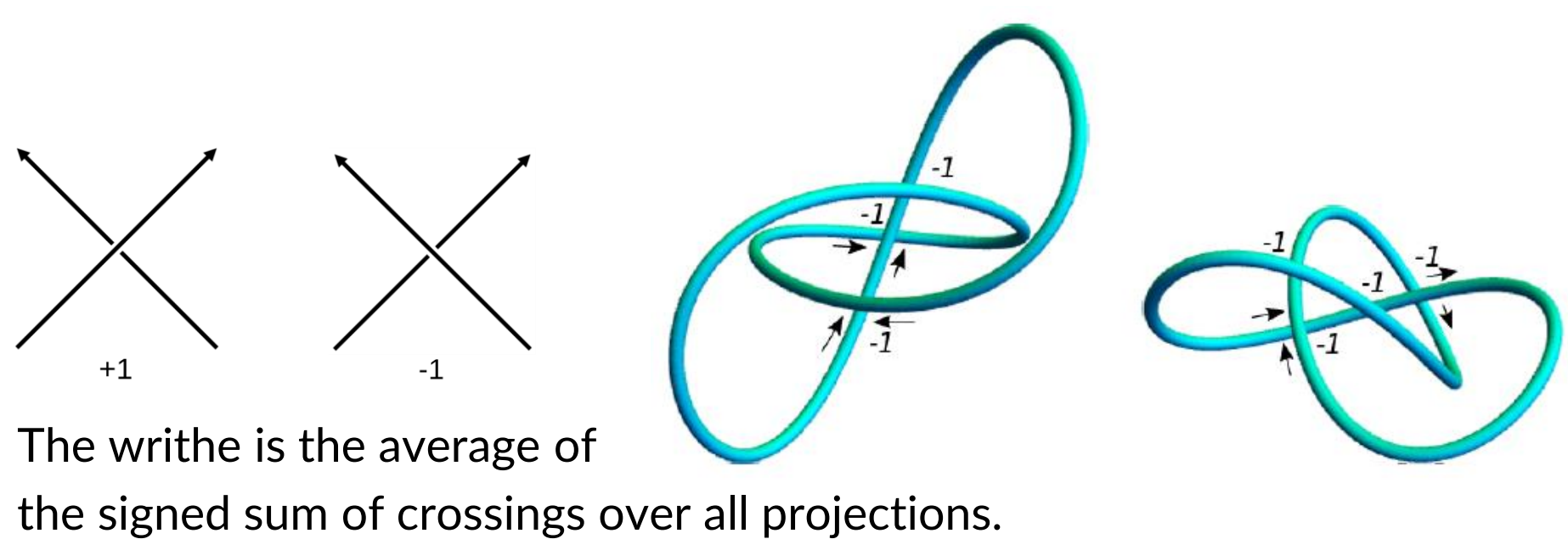


Applications of writhe to protein structure predictions from BioSAXS data

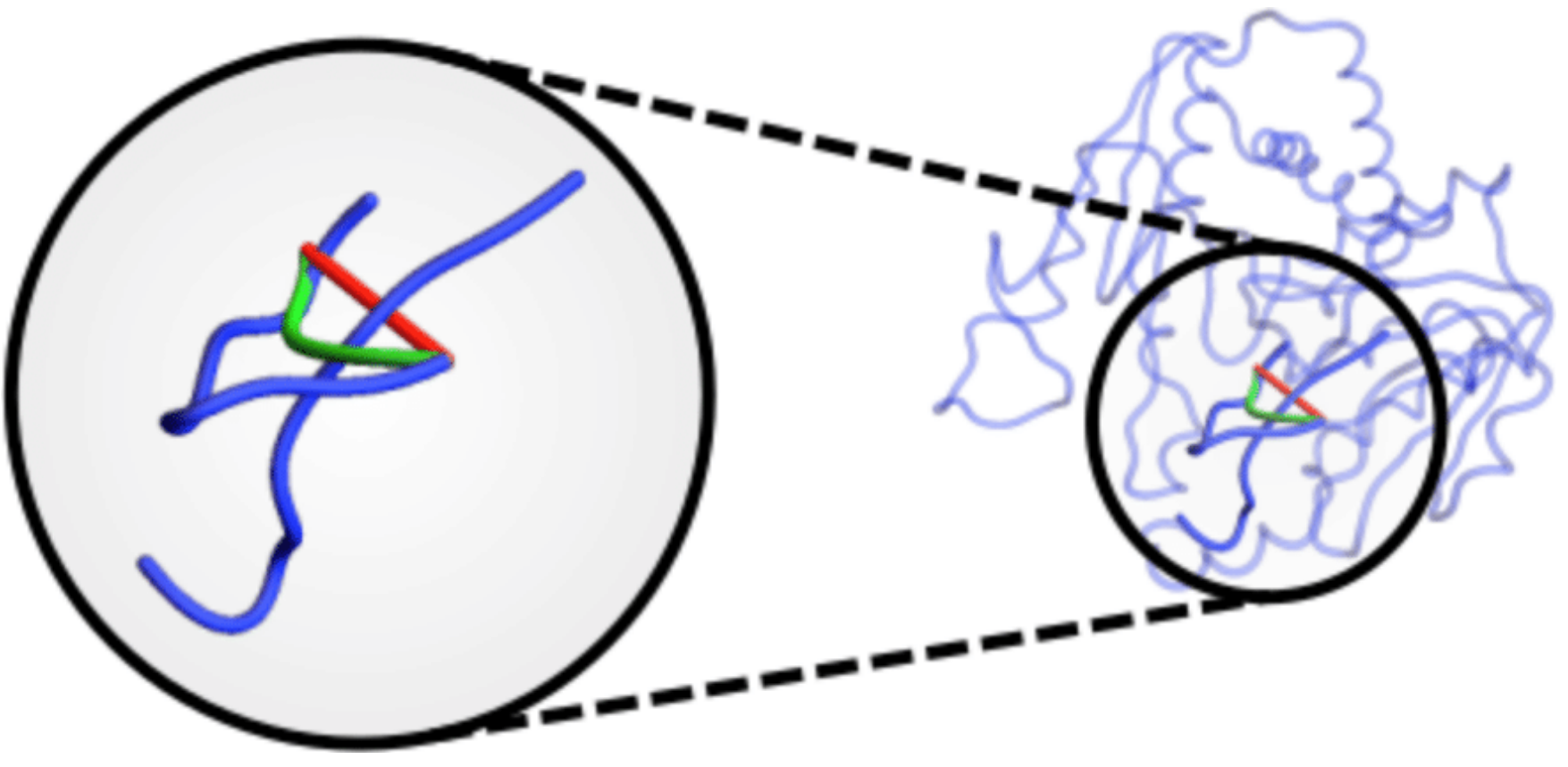
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There is much interest in developing quantitative methods to compare different protein structures or identify common sub-structures across protein families.



METHODS

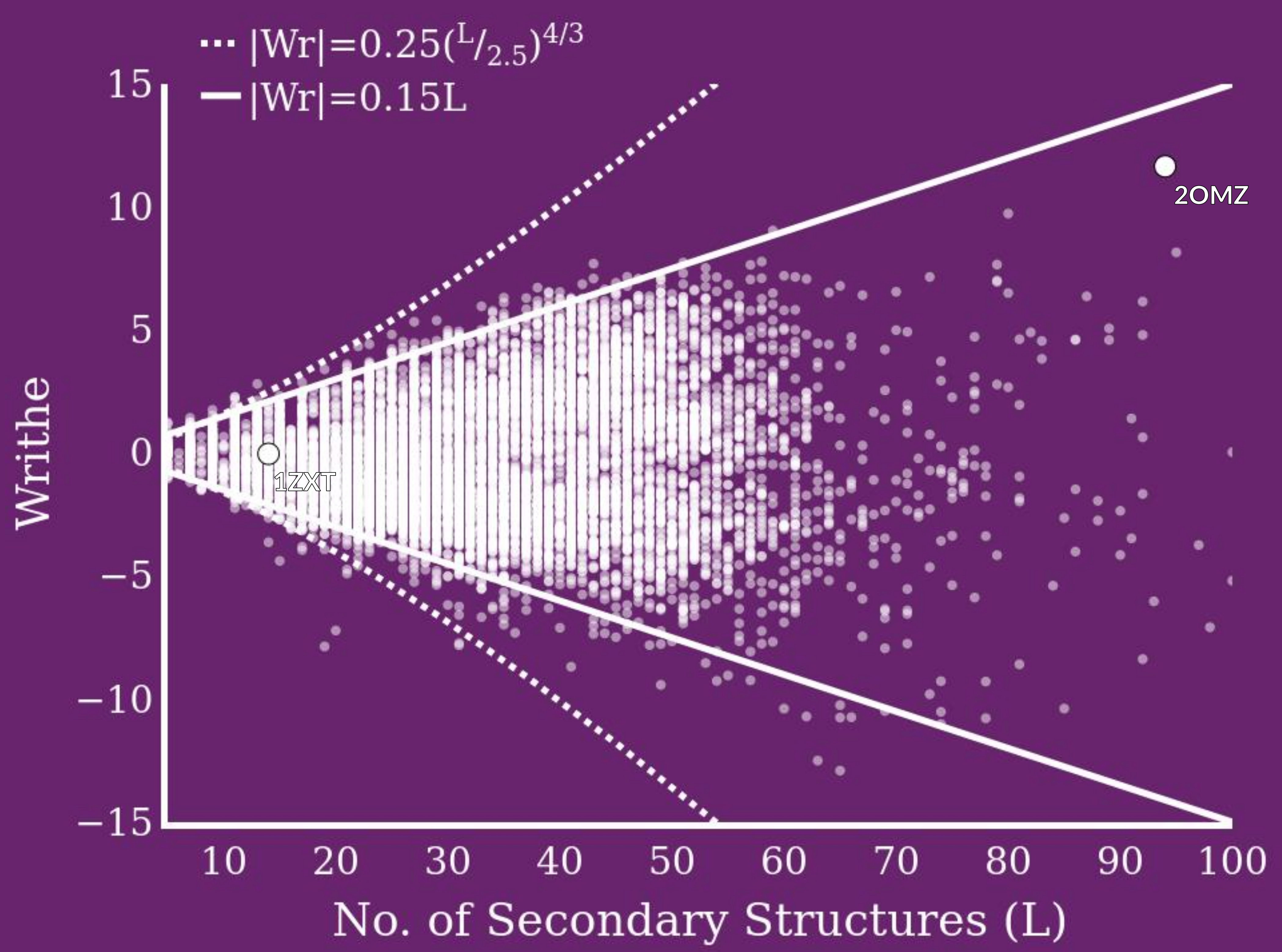
- For a representative sample of >10000 entries to the PDB.
- We compute the Writhe of their smoothed backbone curves.
- We developed the SKMT algorithm to smooth the backbone curves whilst preserving essential crossings.
- Here, the length of a protein is its number of secondary structure elements.



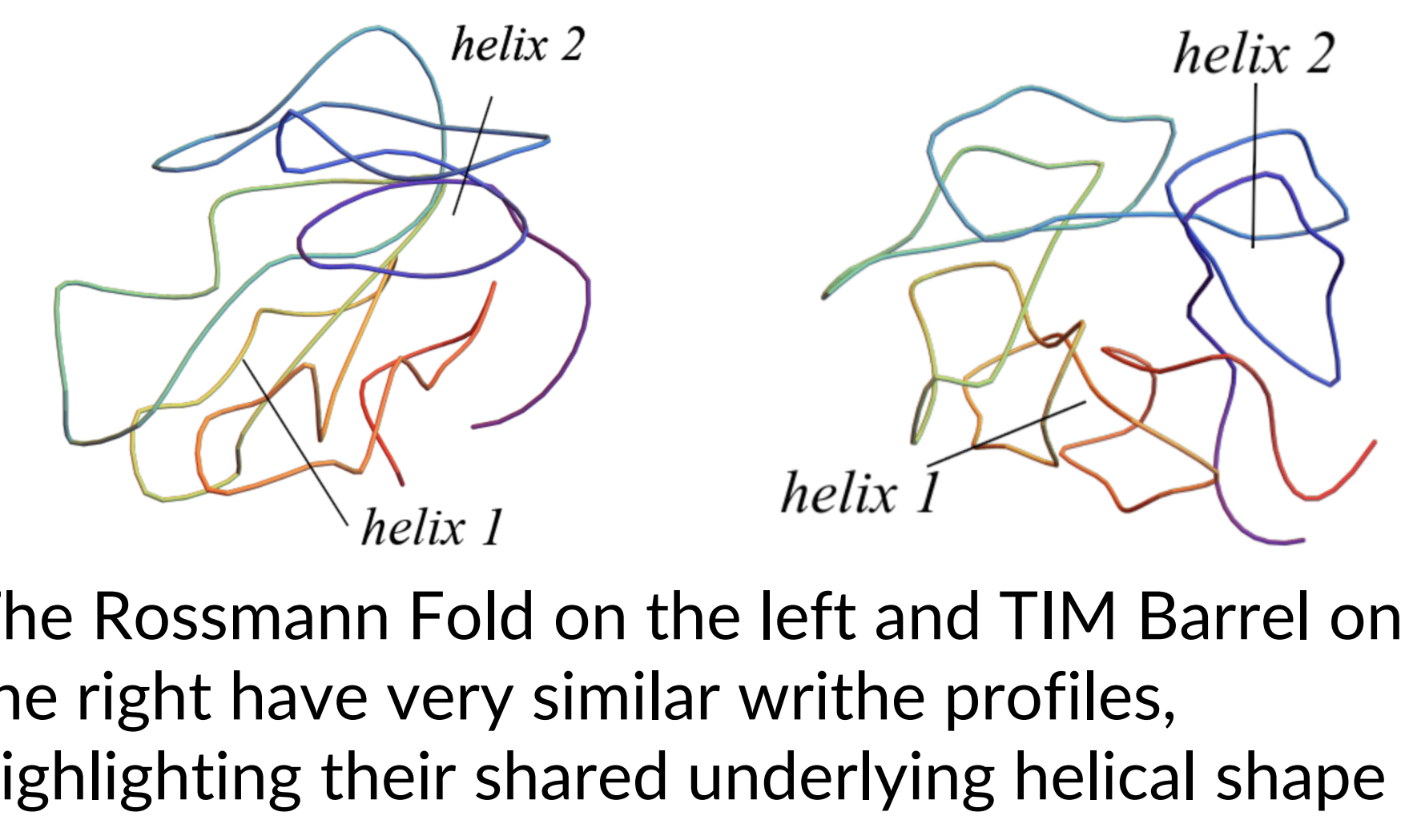
RESULTS

- 97.4% of the data falls within the linear bound 0.15L.
- 99.8% of the data falls within the theoretical knot bound
- Helical structures represent maximal entanglement conformations, providing stability.
- Systematic net zero entanglement conformations exist, though their function is not yet clear.

There is a limit on the amount of entanglement of a protein's backbone



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The Rossmann Fold on the left and TIM Barrel on the right have very similar writhe profiles, highlighting their shared underlying helical shape

