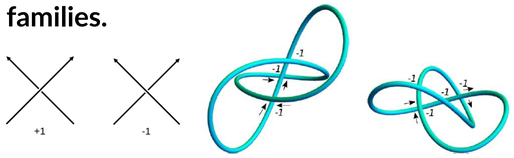
A writhe-based approach to realistic protein structure prediction from BioSAXS data and flexible structure comparison

arron.n.bale@durham.ac.uk

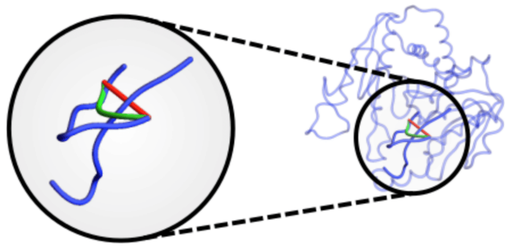
There is much interest in developing quantitative methods to compare different protein structures or identify common sub-structures across protein families.



The writhe is the average of
the signed sum of crossings over all projections.

METHODS

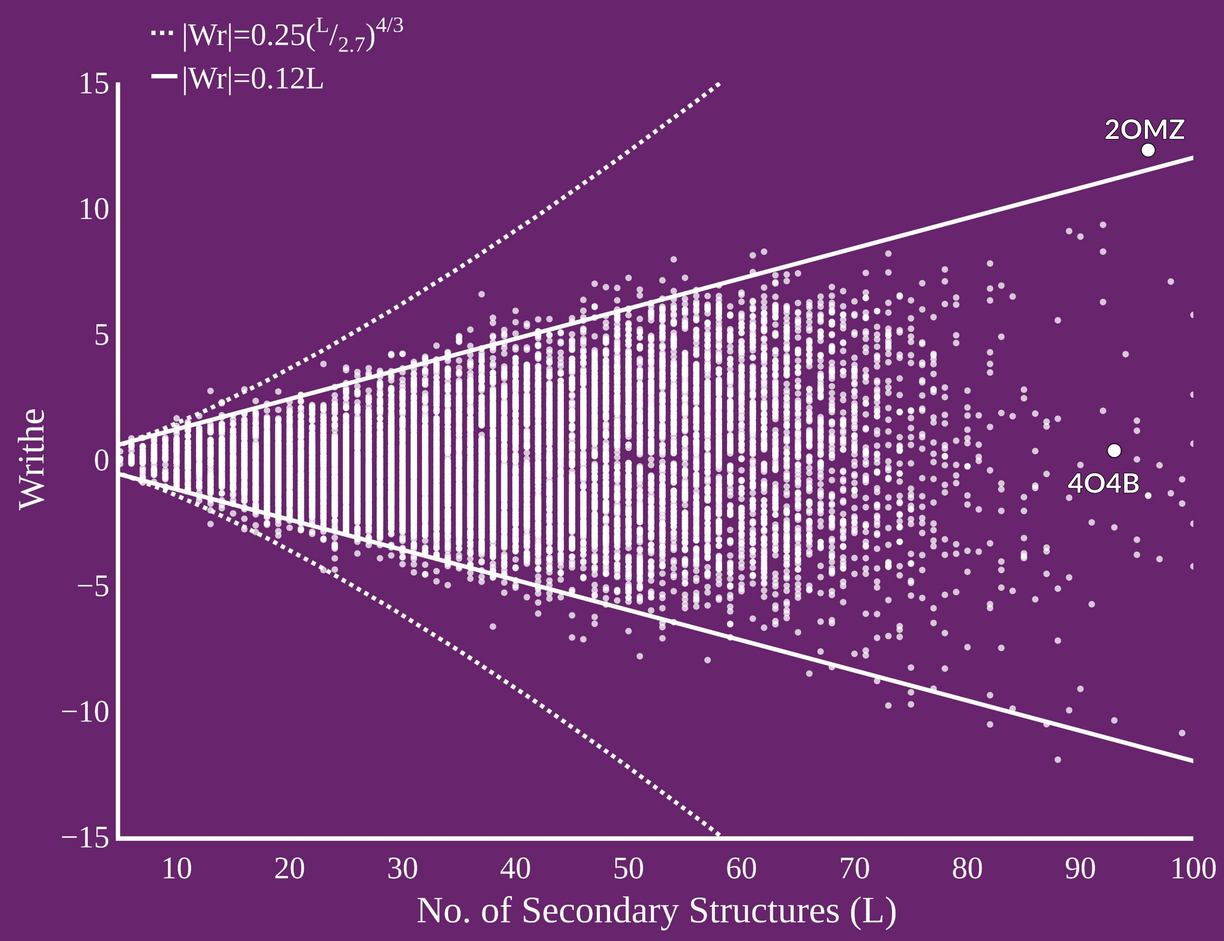
- We took a representative sample of >10000 entries from the PDB.
- We compute the writhe of their SKMT smoothed backbone curves.
- The SKMT algorithm produces a minimal representation of the backbone, preserving essential crossings.
- We define the length of a protein to be its number of secondary structure elements.



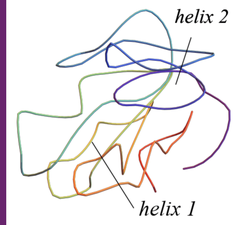
RESULTS

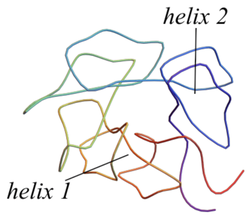
- 97.9% of the data falls within the linear bound 0.12L.
- 99.9% of the data falls within the theoretical knot bound.
- Helical structures represent maximal entanglement conformations, providing stability.
- Systematic net zero entanglement conformations exist, though their function is not yet clear.

There is a **limit** on the **entanglement** of a **protein's backbone** relative to its **secondary structure**

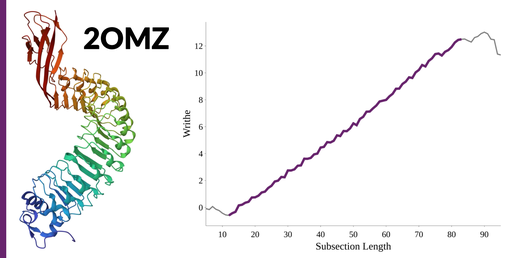


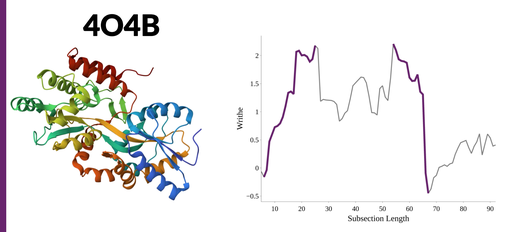
Read the full paper or try out the interactive notebook here

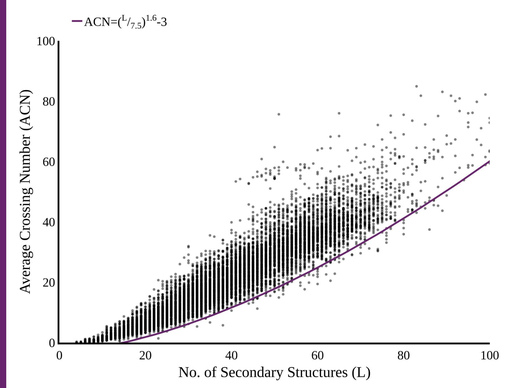


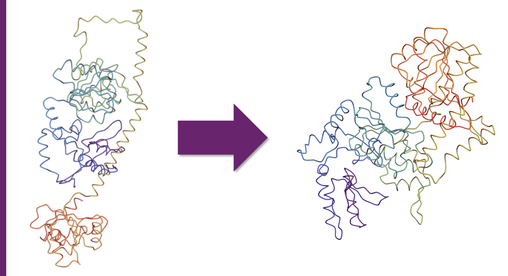


The Rossmann Fold on the left and TIM Barrel on the right have very similar writhe profiles, highlighting their shared underlying helical shape









Arron Bale, Rob Rambo, Chris Prior

Durham University · MoSMed Molecular Sciences for Medicine · diamond