

BCH222 2011 – Suggestions for data-mining projects

Ramachandran-plot related

What is happening in some of the well-defined local details of specific amino-acid plots?

- E.g., for Thr, what are the 4 peaks in the ϕ, ψ β region doing? (Hypothesis: combination of local sidechain-backbone H-bonds, ϕ, ψ prefs, & methyl bumps. Check contacts in examples; compare with Ser & Val.)

How do local sidechain-backbone H-bonds influence ϕ, ψ , rotamers, and local structural motifs?

- For Asn/Asp vs Gln/Glu? (See the unique nature of Asn, and the difference one extra methylene C makes for Gln)
- For Tyr/His Trp? (Look at the "tyrosine corner"; look also at favorable ring packing for Trp)
- Why, for trans Pro, can't C γ -exo pucker occur for the small central datapoint peak in the ϕ dimension? Why, for cis, also not for the α -helix ϕ, ψ peak?
- What is the relative importance of rotamer (esp. χ_1) dependence on ϕ, ψ values versus dependence on secondary structure?
- Same comparison for systematic differences in value of τ (the N-Ca-C angle)?

Rotamer-related

- SS: Define the 5-D rotamer preferences for disulfides (both generic and family-specific)

We've illustrated two clear "decoy" rotamers for Leu (Lovell 2000) – a peak in the distribution that is a systematic fitting error where essentially all cases are incorrect. [Eclipsed 180°-flip cases for Val/Thr/Ile are also "decoys".]

- Are there definable decoy rotamers for Met, where S position is same but reached a different way?
- Are there definable decoy rotamers for Arg, where guanidinium is flipped over in density? Or are there such flipped states where either version could be OK?
- How many H-bonds does it take to stabilize a fully-eclipsed χ angle?
- What rotamers always require changing one or more bond angles $>1\sigma$? Wider or tighter? How much? [Start from the Asn/Asp and Phe/Tyr one mentioned in Lovell 2000.]

File-level questions

- Is it true that structures published in Science/Nature/Cell are worse on average (as claimed in Acta Cryst D paper)? Or is the apparent effect explained by difference in size (as claimed by a later unpublished study)?
- Are structure without deposited data (Structure Factors) worse on average? [Need to compare for dates before 2007, when SF deposition became required.]

Other

- Expand our list of $<1\text{\AA}$ resolution structures where good H atom peaks show in difference map, and use them to study accuracy of amide flips. Or to study some other detailed property.
- Do a more usual BCH222 project on 3D-structure-related aspects of a particular macromolecular system

*** Note: Many would be suitable for working in pairs ***