

# Structural Biology: Assignment 1

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## Abstract

This is an abstract abstract.

## Preface

This is an assignment report in connection to the *Structural Biology* module in the Computational Biology course at the University of Cambridge, Lent term 2017. All related code is as of March 17, 2017 available through a Github repository by contacting [hpa22@cam.ac.uk](mailto:hpa22@cam.ac.uk).

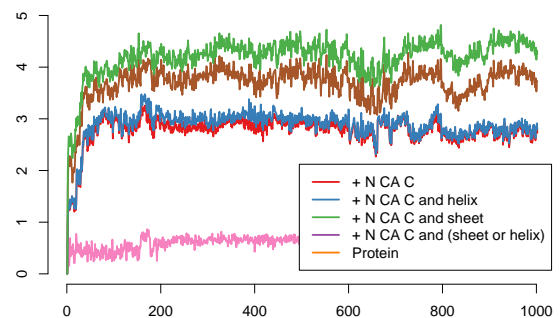


Figure 1: Things

## Exercises

### 1

How would you describe its structure?

The protein in essence consists of a toroidal structure made up by anti-parallel beta-sheets. These are separated into two sub-structures of 6 and 3 beta-strands each. Together, the structure forms a seemingly twisted, tubular form, making it seem like the top conformation is made out to capture incoming molecules of some sort. Even though this might be because of resolution issues, water molecules do not appear to be present within the structure, or at least not frequent. Maybe electrostatically repelled?

In aligning the structures, we can clearly see how the “entrance” to the capturing cavity is inaccessible in the starting structure (i.e. during X-ray crystallography). Aside of the general opening in the structure, the red (opening) appears to have a slightly bigger cavity.

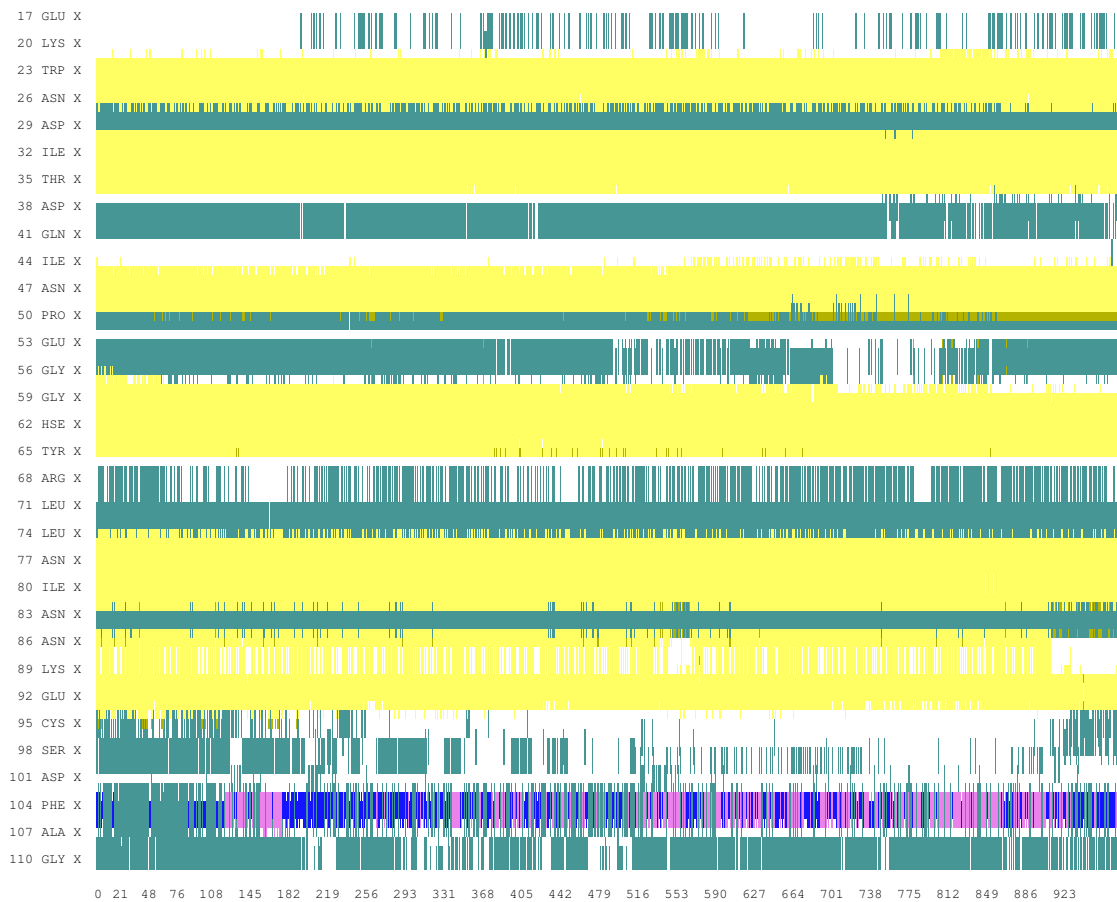


Figure 2: timeline

Formation of new (pink) domains. Amino acid involved in forming helix very variable. Most domains fairly stable overall, but most also alternate at some point.



Figure 3: domainchange

ARG90-XXX120 are the end of one beta-sheet (arrow) and the bottom of another. SER120 is the 3-one (head), whereas ARG90 is the 6-one (bottom).

INCLUDE PINK DOMAIN THINGY

SER27-PRO50 are on the other side of the 3-domain, and

## 0.1 9

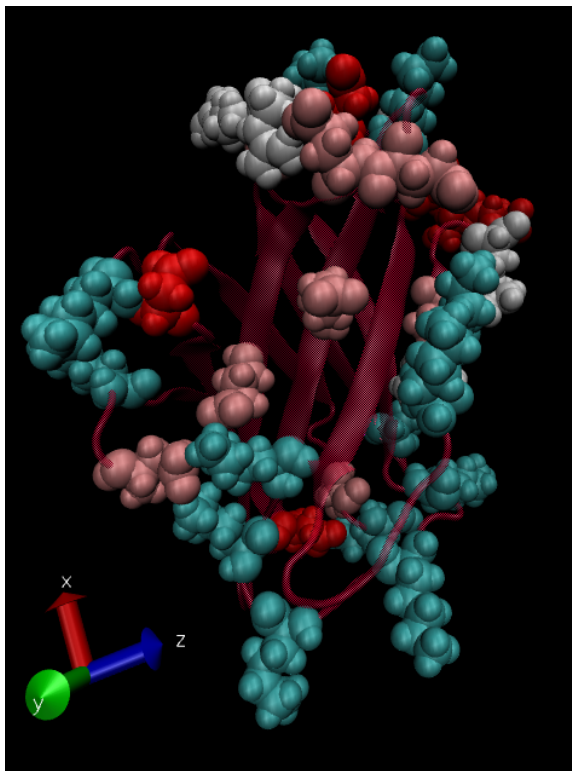


Figure 4: charged

Charged guys are far away from the core structure.

The flexible structures of the protein also tends to consist of smaller amino acids (the spaghetti-like things) (plotting "small" residues)

No ions in complex.

Almost no overlap between polar and hydrophobic amino acids.

## 0.2 10

Non-functional form: Water molecules in cavity.

Functional form: No water molecules in cavity.

## 0.3 11

The molecule stays pretty much the same, with the ring inside of the cavity. In the end, it comes together with the other other side of the cavity. It has also functionally "bent over", i.e. so that it hangs "inwards" from the other side of the cavity. A 180+ degree rotation around it's axis.