

Exercise 2.1

Exploring carbonic anhydrase, 1CA2, and defensin, 1I2V, in Jmol

Download the structure "1CA2" (carbonic anhydrase). Open in Jmol

Secondary structure :

```
select protein
wireframe off
cartoons
color structure
```

Topology:

```
select protein
wireframe off
cartoons off
color group
```

Trace the chain from N to C. On average, how many residues does it take to cross from one side of the protein to the other?

beta sheet :

```
select protein
wireframe off
cartoons off
restrict sheet and backbone
wireframe 0.3
center selected
color cpk
hbonds on
```

How many sheets?_____ How many strands?_____

alpha helix:

```
select protein
wireframe off
cartoons off
restrict helix and backbone
wireframe 0.3
center selected
color cpk
hbonds on
```

How many real alpha helices? _____

View temperature factors (B-values) :

```
select protein
wireframe off
cartoons
wireframe 0.3
center selected
color temperature
hbonds off
```

Higher B is red, lower is blue.

View backbone only:

```
wireframe off
backbone 1.0
```

Where are the minimum _____ and maximum _____ B-value?

NMR structure

Download the structure "1I2V" (defensin). Open in Jmol

```
select protein
wireframe 0.2
model 0
color group
```

```
wireframe off
backbone 1.0
```

Tools/Animate/Loop

Where in the structure is the greatest disorder/uncertainty?
