Exploring Sequence-Structure Relationships
with UCSF Chimera

- Demonstration (~20 mins):
  - preview of some of the tools you will be using
  - OK (preferable?) to watch rather than trying to follow along; if you do try things, close session or quit/restart before starting the tutorial
- Hands-on tutorials:
  - **Sequences and Structures** (~25 minutes)
  - **Superpositions and Alignments** (~40 minutes)


Combining Structure with Other Data

- Structure provides spatial information
- Sequence adds non-spatial information
- "The whole is greater than the sum of the parts"

Demonstration Outline

Basic sequence-structure crosstalk:

- **Sequence** shows the individual sequences of structure chains
- selecting in sequence selects structure and vice versa
- pastel boxes show helix and strand assignments
- mouse over sequence reports structure residue name/number
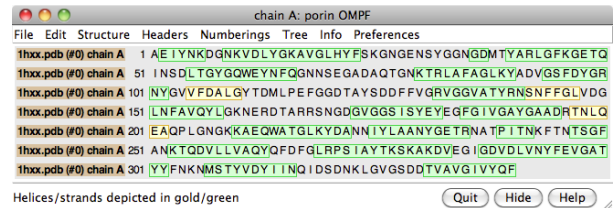
Multiple sequence alignment from a file:

- external sources include many other programs and databases; example is from PFAM
- shown with **Multalign Viewer** (actually same tool as **Sequence**)
- sequence-structure association is automatic, tolerates some mismatches
- many appearance settings (**Multalign Viewer** preferences)
- lines of information above the sequences are "headers"
- numerical headers are automatically assigned as residue attributes of associated structures
- many options for calculating **Conservation** header (**Multalign Viewer** preferences)
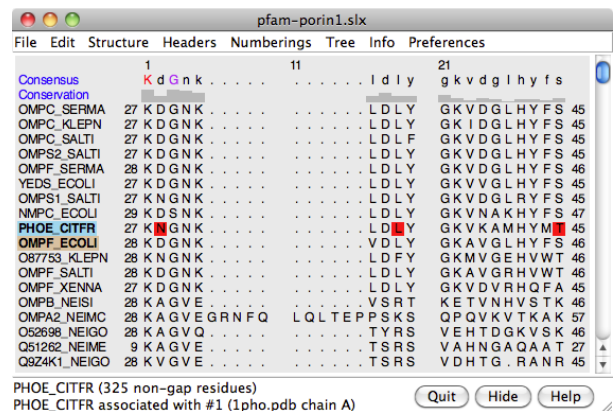
When multiple structures are associated with an alignment:

- structures can be superimposed based on the sequence alignment
- **RMSD** header shows "spatial conservation"
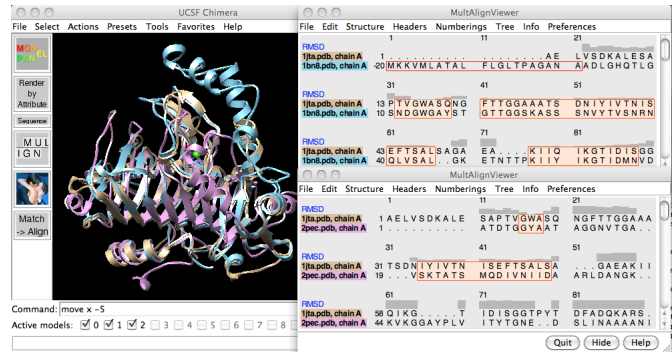
Creating sequence alignments in Chimera:

- **MatchMaker** creates pairwise sequence alignments which are then used to superimpose the structures
- given a multiple structure superposition (regardless of how it was made), **Match→Align** creates a multiple sequence alignment
- sequence alignments can be saved in many formats, those that can be read plus EPS