Preparing Your Structure

Production Runs

Why?

- Structures from PDB are not perfect
- Rosetta may fail
- Garbage in garbage out
  - Wrong answer
- Benefits
  - Less time spent on paths spent on re-relaxing the same errors of the input
  - Less noise
  - Lower scores

What to Do?

Answers from the Developer Community

- Clean the structure
- Repack the structure
- Relax the structure

The Meiler Lab Philosophy

- Clean PDB with clean_pdb.py
- Run Relax

clean_pdb.py

What it does!

- Removes HETATM
- Changes names of phosphorylated residues so Rosetta understand them (SEP -> SER)
- Removes multiple conformations of residues
- Renumbers pdb starting at number 1
- Preserves only ATOM lines
- Rosetta adds hydrogens

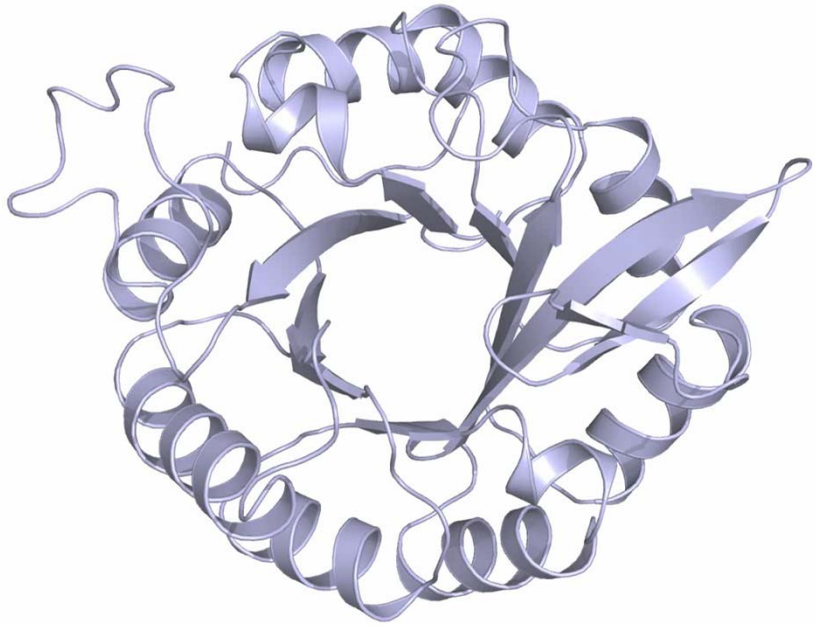
What it does **not** do!

- Rebuilds missing coordinates (see loop building tutorial)
- Make everything ok.

```
python clean_pdb.py -h
```

What is Relax?

- Simple structural refinement
  - Removes clashes
  - Puts model in energy minima
- Sample through Monte Carlo movements of backbone
- Method to generate multiple conformations of a model

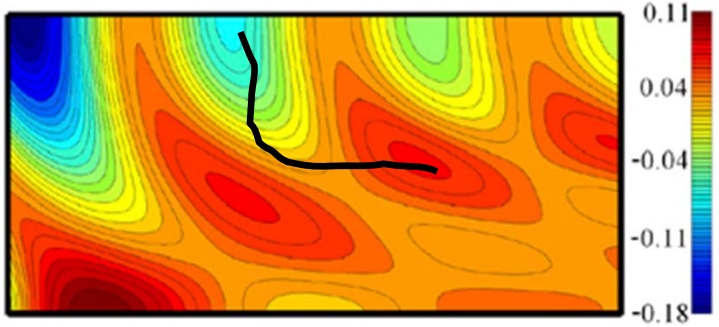


Design, Ligand Docking, Protein-Protein Docking
Structure Preparation

- You need multiple models!
- Obtain models through relax
- Use top 1-10% by score

```
relax.linuxgccrelease –database
<database> -s <structure> -ex1 –
ex2
–relax:sequence –nstruct 100
```

MD Conformational Sampling



Monte Carlo Conformational Sampling