In class exercise:
Ramachandran plot
Superposition
Crystal contacts
Ramachandran Plot matches stats of good Xray structures

Ramachandran used a physical model of dipeptides to determine the allowed (dark) and disallowed (white) combinations of phi and psi backbone angles. The observed frequencies roughly agree with R’s allowed regions.
Ramachandran plot in Coot

Read in **7dfr.pdb**
Validate > Ramachandran plot

- Click to identify residue
- Plot changes to match residue type
- Helps to identify outliers, poorly modeled residues
- Find a glycine.
- Find a proline.
Showing symmetry in Coot

Draw > Cell & Symmetry
   Master switch: Yes
   Show unit cells: Yes
   Symmetry by molecule:
      Display as CAs, Color by symop
Draw > Cell & Symmetry
Symmetry by molecule:
Display near chain, Color by symop

trigonal space group!
Find crystal contacts

Crystal contacts are locations where atoms are close to atoms of a symmetry-related molecule. (Can be non-crystallographic symmetry)

Play a role in crystal formation.

May be distorted by the interaction energy.

Click to label atoms in crystal contact

S138, C152, F140, D142
Find crystal contacts

Draw > Cell & Symmetry
Symmetry by molecule:
Display sphere, standard colors

Use control-leftmouse-drag to pan.
Superposing two molecules in Coot

- Superposition
  - ...requires a sequence alignment.
  - ...solves for rotation/translation by least-squares

\[
\sqrt{\frac{(M r^a_i - r^b_i)^2}{N}} \quad \text{... to solve for } M
\]

\( r^a_i \) and \( r^b_i \) are the coordinates of the \( i \)th residue (more precisely, the two residues in \( i \)th column of a sequence alignment) of molecules \( a \) and \( b \) respectively.
Superposing two molecules in Coot

Read in 7dfr.pdb (if not already)
Read in 4m6k.pdb

**Calculate > SSM superpose**
select chain A for both

**Display manager**
CA+Ligs SecStr Col

Later, try...

**Display manager**
Jones Rainbow
Model quality metrics

- Resolution
- R-factor (free R-factor)
- Overall B-factor (approx Wilson B)
- Quality of density (holes in rings, H bumps)
- Ramachandran plot
- Rotamers
- other stereochemistry (bond lengths, angles, chirality)
- B-factors
- Rsym, completeness (measure quality of data, not of model, but related)
Comparing models

Questions you ask when comparing two models:
- How similar?
- What method was used? (Xray, NMR, cryoEM, homology)
- Where are the differences?
- How significant are the differences?
- What may have caused the differences?
- Any differences in function?

metrics and factors
- RMSD
- sequence differences, insertions/deletions
- ligands
- crystal contacts
- relative model quality (see previous slide)