Exercise 4.1. Make a beta hairpin

Make sure the hydrogen bonds are of the anti-parallel type, with nearly perfect distances. All Valines should be on the same side of the sheet.

Edit | Build | Protein, Geometry: **anti-strand**. Residue: **ADVDVKVSPNGVEVKVRA**

Zoom out.

Select half of the chain above the Glycine. Move it (**shift-alt-middlemouse**) so that the valines are lined up on the same sides of the backbones.

Hide side chains

Edit/Potential/Restrain.
Set Target 1.8, 1.8, Weight 100. Select H and O atoms from paired Valines.
Set Target 2.8, 2.8, Weight 100. Select N and O atoms from paired Valines.

Compute | Prepare | Structure preparation. **Correct** if necessary. **Protonate3D**.

SVL: run 'gizmin.svl'.

If there are errors in the restraints, **Cancel/GizMOE,** open **Potential Setup** (extreme lower left of the MOE window). **Restraints**. Click on restraints and delete or modify.
Restart **SVL: run 'gizmin.svl'.**

Look at out the structure. Does it have beta pleating? (paired sidechains? 2-up, 2-down?)
Is the hairpin a beta turn? (residues SPNG. Check agains lecture 6 slides.) What type?

Cancel/GizMOE . Remove the restraints. Restart **SVL: run 'gizmin.svl'**.

Does the structure hold together or fall apart?

Save MOE file. Upload to the homework server. Be sure to check exercise4.1