

Exercise 5.1. 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/Restraining. 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/Structure preparation. **Correct** if necessary. **Protonate3D**.

GizMOE/Minimize.

If there are errors in the restraints, **Cancel/GizMOE**, open **Window/Potential** setup. **Restraints**. Click on restraints and delete or modify. Restart **GizMOE/Minimize**.

Look at out the structure. Does it have beta pleating? (paired sidechains 2-up, 2-down)
Is the hairpin a beta turn? (residues SPNG)

Cancel/GizMOE . Remove the restraints. Restart **GizMOE/Minimize**.

Does the structure hold together or fall apart?

Save MOE file. Upload as Ex5.1. Write comments here: