Creating a peptide bond between two protein structures in Chimera

This tutorial shows the step-by-step procedure to join two protein structures via a new peptide bond in the Chimera software. A few checks are necessary beforehand.

Both proteins must contain the N/C-terminal nitrogen and carbon atoms to be joined. Some structures available at the PDB may be lacking these atoms. If that is the case, use a command such as *swapaa* (to replace the first or last residue) or *addaa* (to add N/C-terminal residues, useful if you intend to have a linker region) to correct the structure file. All of this is done in Chimera.

Be acquainted with Chimera syntax to select the correct atoms. For example, entering the following in *Select > Atom Specifier*:

#0:129.B@C

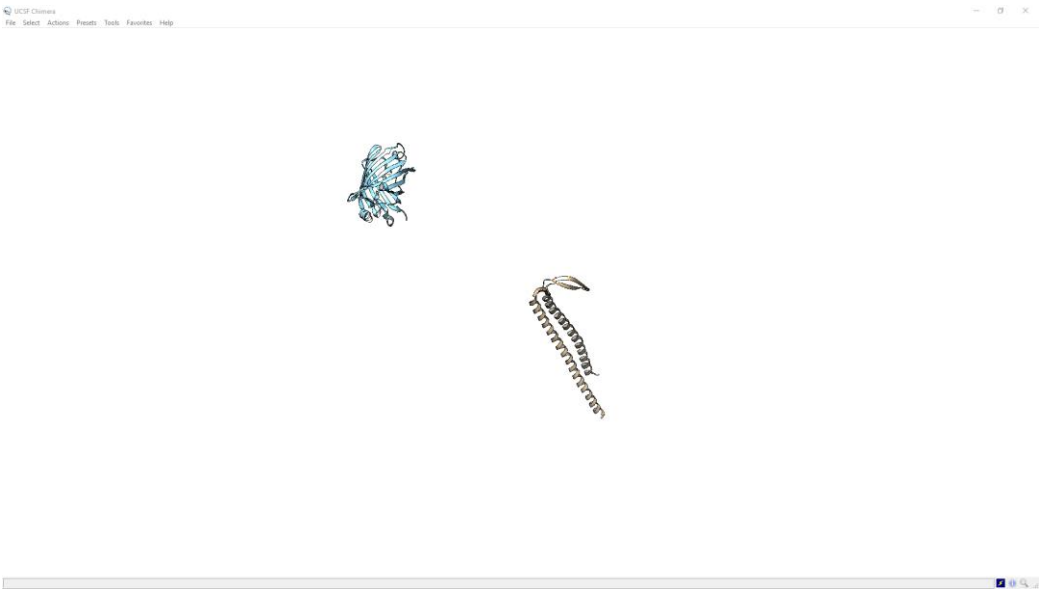
Means “select atom C in residue 129 of chain B in structure model 0”.

(model number)
: (residue number)
. (chain name)
@ (atom name)

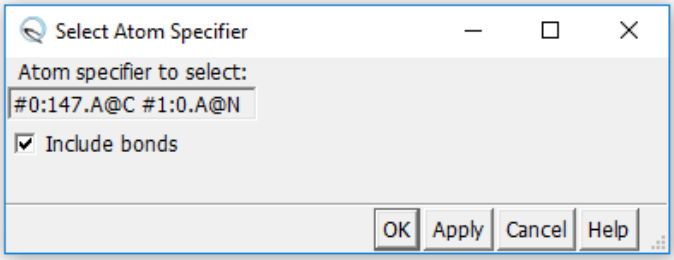
Bear in mind “C” is the name of the atom, not the element. Other carbons in the same residue will have names such as “CA”, “CB”, etc. By convention, the carbon contained in the peptide bond is named just “C” and the nitrogen is named “N”. But if something goes wary, check if the nomenclature in your .pdb file is different.

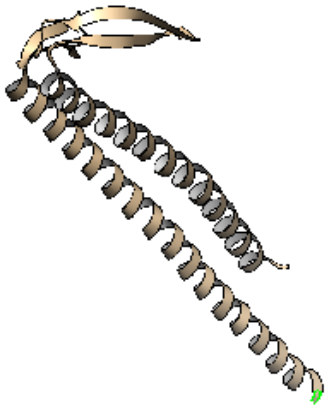
Here is the step-by-by step procedure to fuse the gPFD structure to the YFP (Venus) structure in Chimera. The fusion will be done at the C-terminus of gPFD.

1. Open both .pdb files in the same Chimera session. The first model to be opened will be numbered 0, and the next will be numbered 1.



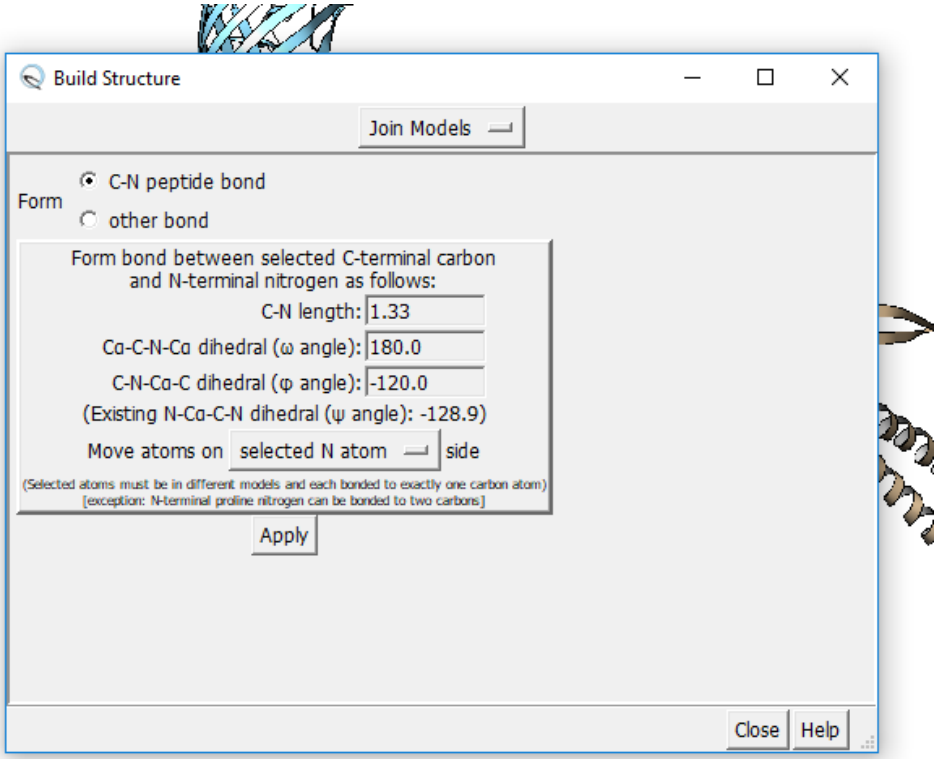
2. Using *Select > Atom Specifier*, select the C-terminal carbon of gPFD and the N-terminal nitrogen of Venus. Since gPFD was opened first (model 0) and Venus was opened next (model 1), the command will look like this: #0:147.A@C #1:0.A@N – a little unusual, but the first residue in the Venus structure is numbered “0”.





Note that the N/C-terminal residues of Venus/gPFD are now highlighted. If the representation was set to showing all atoms instead of ribbons, the exact selected atoms would be highlighted.

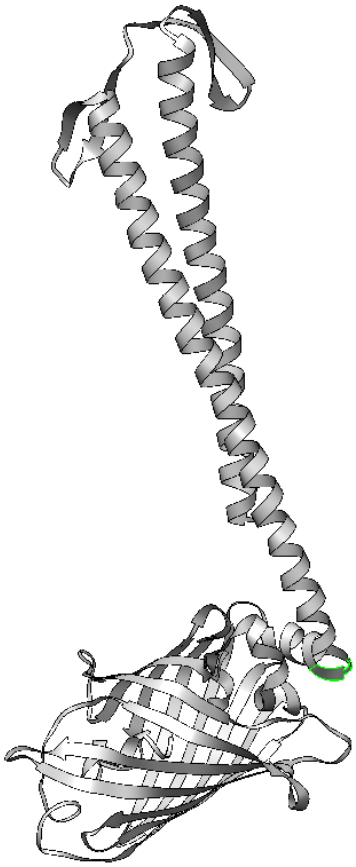
3. Open *Tools > Structure Editing > Build Structure*
4. In the top drop-down menu of the new window, choose *Join Models*.
5. Tick *C-N peptide bond*



The *Apply* option will only be available if two "compatible" nitrogen and carbon atoms have been selected (sometimes I need to untick and re-tick the *C-N peptide bond* option). This prevents mistakes but the action is irreversible.

6. Modify the bond properties if desired. Bond angles can be changed later in *Tools > Structure Editing > Build Structure* and then *Adjust Torsions* or *Adjust Bond Angles* in the drop-down menu.
7. Choose whether you want to move Venus to the end of gPFD (i.e. gPFD stays in place) or conversely. To move Venus, leave the drop-down menu at "selected N atom" (since the selected nitrogen atom is in the Venus structure).

8. Hit *Apply* and hope for the best.



As you can see, this results in some clashes where the structures were joined. This can be either fixed by adjusting bond angles or prevented by including a linker sequence (e.g. using the *addaa* command). It's also much easier to adjust angles in linker sequences since they are meant to be (and look) unstructured.