Term project guidelines

How to regenerate 3-fold symmetry from a monomer-monomer interface design

When you have completed an interface design that includes one monomer of your trimeric ligand and one RBD domain, then you can copy the designed interface to the other two positions as follows.

1. Let's say your timer ligand has chain names "A" , "B", and "C" and you designed "A".
Drag the designed monomer "A" and RBD (single domain) chains together. If you added waters consolidate them into one chain (Join chains) and drag that chain next to the "A" and RBD monomer. Group under one tag, such as "design A".

2. Copy tag "design A". Paste twice. Name the other two tags "design B" and "design C".

3. Superpose "design B" on "B" : Select "design B". Unfix. Select "B". Fix. in SEQ: Alignment panel, select tag "design B". Set to alignment group A. Select "B". Set to alignment group B. Select all other chains. Set to alignment group i (ignore). Make sure Options... 'Move all other atoms in Tag', is checked. Superpose. RBD and ligand monomer shift to position B.

4. Same as 3, for "C".
Superpose "design C" on "C" : Select "design C". Unfix. Select "C". Fix. in SEQ: Alignment panel, select tag "design C". Set to alignment group A. Select "C". Set to alignment group B. Select all other chains. Set to alignment group i (ignore).
Make sure Options... 'Move all other atoms in Tag', is checked. Superpose. RBD and ligand monomer shift to position C.

5. Delete the undesigned originals. Keep the "design" tags. Delete any other RBDs that you are not using.

6. Select all three tags "design A", "design B", and "design C". Unfix. Fix other atoms. Hilight the termini of the RBDs and the fusion domain. Use Measure to draw distances between connected terminal residues. Clear selections. Select all "design" tag and move them together to minimize the distances. Done.