**<Section|Structure Preparation>**

This considers {mouse and rat| examined organisms}.

1. We initially perform the {sequence alignment|stage} by generating {GluN1,GluN2,GluN3| sequence alignment }. {MAAFT Server| Software }[[1]](#footnote-0) {7|version} is used for the alignment using {default|settings}.
2. Next, perform {alignment refinement|stage} using {GLProbs|software}. Apply {2|consistency transformation passes}, followed by {100|iterative refinement passes}.
3. A {manual sequence alignment|stage} is later needed using the {result of previous step| base template }. The first uses {GluN2DLBD|template structure } with {3OEK|PDB ID}. The second uses {GluN3BLBD|template structure} with {2RCA|PDB ID}. Use {BioLuminate package|software} for this alignment. This procedure is necessary to account for insertions and deletions present in the template structures.
4. <for each| generated pose>, perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å| target criteria}. Subsequently, {optimization|operation } is also performed on {side chain rotamers|(optimization) target}.
5. <while|pH|lte|7>[[2]](#footnote-1), perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å| target criteria}. Subsequently, {optimization|operation} is also performed on {side chain rotamers|(optimization) target}. Iterate over <+|1>[[3]](#footnote-2).
6. <if|pH|lte|7 >[[4]](#footnote-3), perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å|target criteria}. Subsequently, {optimization|operation} is also performed on {side chain rotamers|(optimization) target}.
7. <else if|pH|between**|[8-12]**>[[5]](#footnote-4), perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å|target criteria}. Subsequently, {optimization|operation } is also performed on {side chain rotamers|(optimization) target}.
8. <else>[[6]](#footnote-5), perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å|target criteria}. Subsequently, {optimization|operation } is also performed on {side chain rotamers|(optimization) target}.
9. <for|pH|**[1-7]**|+|1>[[7]](#footnote-6), perform {energy minimization|operation}. This operation is done on the {receptor residue|(minimization) target}. This is applied to any residue {lte 5  Å|target criteria}. Subsequently, {optimization|operation} is also performed on {side chain rotamers|(optimization) target}.

1. Katoh, K., Rozewicki, J. & Yamada, K. D. MAFFT online service: multiple sequence alignment, interactive sequence choice and visualization. Brief Bioinform, https://doi.org/10.1093/bib/bbx108 [↑](#footnote-ref-0)
2. <while|key|logical operator|value> [↑](#footnote-ref-1)
3. <operation|value> [↑](#footnote-ref-2)
4. <if|key|logical operator|value > [↑](#footnote-ref-3)
5. <else if|key|logical operator|value> [↑](#footnote-ref-4)
6. This ideally should provide a link to the previous step (the corresponding if or else if), but this would hurt the readability. [↑](#footnote-ref-5)
7. <for|key|[range]|iteration\_operation|magnitude> [↑](#footnote-ref-6)