**<Pre-step information>**

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-1) {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 {<=5  Å| target criteria}. Subsequently, { optimization|operation } is also performed on {side chain rotamers|”optimization” target}.
5. <while|key|logical operator|value >, perform {energy minimization|operation}. This operation is done on the {receptor residue|”minimization” target}. This is applied to any residue {<=5  Å| target criteria}. Subsequently, { optimization|operation } is also performed on {side chain rotamers|”optimization” target}. Iterate over <operation|key|value>.
6. <if|key|logical operator|value >, perform {energy minimization|operation}. This operation is done on the {receptor residue|”minimization” target}. This is applied to any residue {<=5  Å| target criteria}. Subsequently, { optimization|operation } is also performed on {side chain rotamers|”optimization” target}.
7. <for|key|(range)|increment >, perform {energy minimization|operation}. This operation is done on the {receptor residue|”minimization” target}. This is applied to any residue {<=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-1)