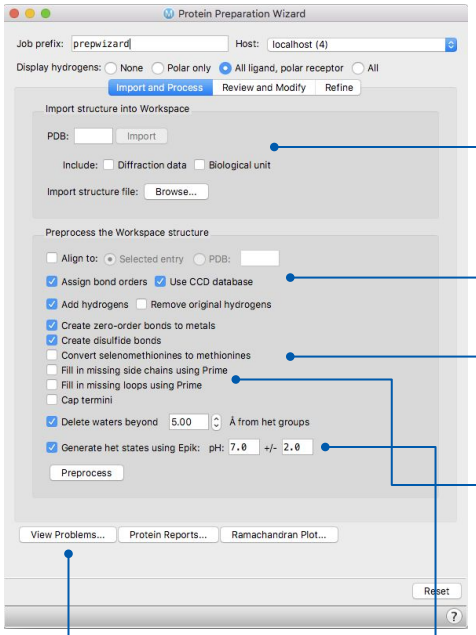
Protein Preparation Wizard

1. Import and Process



Import a structure from the PDB, optionally import the associated diffraction data and biological unit

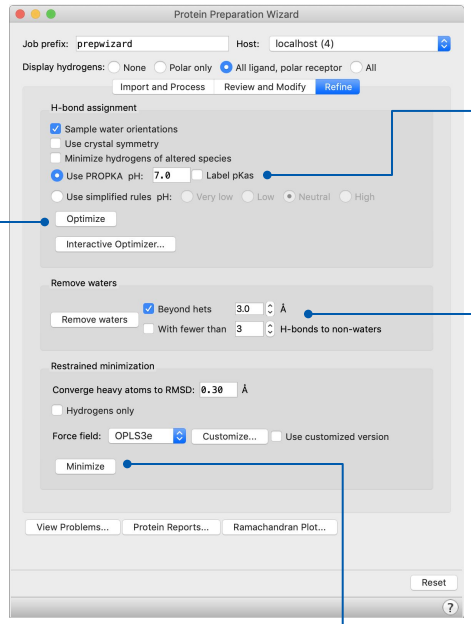
*These setting are **almost** always kept as the default during protein preparation*

Using Prime increases preparation time. The 'Filling in missing loops using Prime' setting is only recommended for loops ≦5 residues

Make sure that pH set for generating your het (i.e. non-protein groups as defined by the pdb file) states agrees with the pH of the system being considered

Click to get a quick sense of how extensive of a preparation is needed for your structure

3. Refine



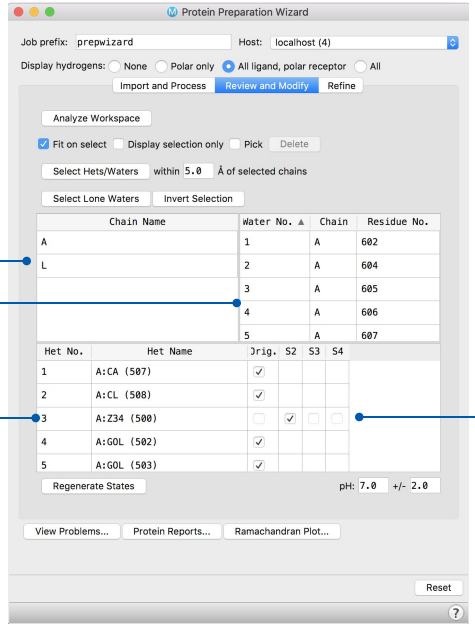
This will address any atom overlapping that have resulted from the addition of hydrogens during the pre-processing step

Make sure that pH set for generating your hydrogen bond assignments agrees with the pH of the system being considered

There is no single best practice for handling waters during protein preparation. Recommendations are highly dependent on the modeling task that you wish to perform with your prepared structure (see Knowledge Base Article 31 for information on preparing structures for Glide docking)

This should be considered as more of a relaxation than a true minimization (not necessary if the structure will be an input for a Desmond MD calculation)

2. Review and Modify



*Select het groups in the chart to zoom into them in the Workspace. Chains, waters, or het groups can also be deleted by clicking **Delete***

Toggle through the possible protonation and tautomeric states for your het groups. The ones checked by default were found to be the most energetically favorable by Epik

Tip
Use the Protein Reliability Report to better assess the quality of your structure before and after preparation