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Reconstructing Solvent Density of Myoglobin Unit Cell from Proximal Radial Distribution Functions of Amino Acids[1] MADELINE GALBRAITH, Duquesne University, GC LYNCH, BM PETTITT, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch —
Understanding the solvent density around a protein crystal structure is an important step for refining accurate crystal structures for use in dynamics simulations or in free energy calculations. The free energy of solvation has typically been approximated using an implicit continuum solvent model or an all atom MD simulation, with a trade-off between accuracy and computation time. For proteins, using precomputed proximal radial distribution functions (pRDFs) of the solvent to reconstruct solvent density on a grid is much faster than all atom MD simulations and more accurate than using implicit solvent models. MD simulations were run for the 20 common amino acids and pRDFs were calculated for several atom type data sets with and without hydrogens, using atom types representative of amino acid side chain atoms. Preliminary results from reconstructions suggest using a data set with 15 heavy atoms and 3 hydrogen yields results with the lowest error without a tradeoff on time. The results of using precomputed pRDFs to reconstruct the solvent density of water for the myoglobin (pdb ID 2mgk) unit cell quantifies the accuracy of the method in comparison with the crystallographic data.

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