A new 3D visualization method with application to histidine in myoglobin

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A protein is commonly visualised as a discrete piecewise linear curve, its backbone geometry being characterised in terms of the extrinsically determined Ramachandran angles. However, in addition to the extrinsic geometry, the protein backbone has also two independent intrinsic geometric structures determined by the peptide planes, and the side chains and their relative orientations. We develop a novel methodology for analysis and 3D visualisation of protein structure, based on the construction of a series of orthonormal coordinate frames, along the protein side chains, and mapping the atoms positions onto a unit sphere. Thus, we obtain a consistent picture of side-chain covalent bonds spatial orientations, though from a different perspective — that of an observer, who climbs up the side chains from one carbon atom to the next. We validate the method by studying the distribution of distal and proximal histidine, as well as of valine in the molecule of myoglobinin, on a statistical sample of all myoglobin entries from PDB (Protein Data Bank) with resolution better than 2.0 Å. The obtained results are in a good agreement with the biological data.

Going beyond traditional visualization schemes that step on laboratory frames, our novel 3D visualization method can be employed as a valuable visual tool for protein side chain construction as well as structure validation and refinement, complementary to widely used visualisation suits like VMD, Jmol, PyMOL and others.

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