Adapting to varying resolutions in ISOLDE

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As the (local) resolution of your dataset degrades, the amount of prior knowledge you need to apply in order to build a reliable model increases. With atomic-resolution data we only really need to know about atoms and how they bond to each other. At intermediate resolutions we need to incorporate knowledge about the chemical identity of the structure (protein/nucleic acid sequence, expected ligands, sidechain compositions) and the finer details of molecule structure such as bond lengths, angles and torsions. At these and lower resolutions it also helps enormously to consider the non-bonded interactions between atoms. At very low resolutions, where helices devolve into featureless sausages and beta sheets become largely uninterpretable, often our only hope is to rely on the pre-existence of higher-resolution models of the same or closely-related domains to provide the overall tertiary structure. In this talk I will discuss how these challenging intermediate-to-low resolution cases can be handled in ISOLDE.