Quantifiying resolvability of atomic features in cryo-EM maps using Q-scores

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Q-scores are calculated locally for individual atoms in a model fitted or built into a cryo-EM map. They can be averaged over groups of atoms to represent resolvability of larger features such as residues in proteins, nucleotides in nucleic acids, and ligands. Plotting of residue or nucleotide Q-scores helps to identify which parts of a model are resolved in the map, and which parts may be unresolved or may need further refinement. A useful property of Q-scores is that for well-fitted models, they correlate strongly to the resolution of the map estimated by FSC; this answers the question 'what is a good score' for a map at a certain resolution. Several examples and related structural insights are shown with models and maps ranging from 2 to 5Å resolution. The connection between Q-scores and atomic B-factors is also explored. Finally, Q-scores are used to help detect and assess water and ion molecules in maps at 3Å and higher resolutions.

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