Validating near atomic and atomic resolution cryoEM structures of molecular complexes

Wah Chiu, Greg Pintilie, Kaiming Zhang, Shanshan Li, Michael F. Schmid

Department of Bioengineering, Stanford University, Stanford, California, and Division of CryoEM and Bioimaging, SSRL, SLAC National Accelerator Laboratory, Stanford University, Menlo Park, California, USA

CryoEM has become a routine tool for 3-D structure determination of single particle with molecular weight of 40kD and above with a resolution ranging from 1.5 and 4.0 Å. There are different challenges to validate the maps and models because of a number of factors: (i) a single specimen can yield multiple structures due to compositional and conformational heterogeneity, (ii) the structure resolution of a cryoEM map is generally not uniform throughout the volume, and (ii) the apparent resolvability of density varies depending on the atom type, extent of inherent flexibility, radiation sensitivity and local chemical environment. We have developed a quantitative parameter (Q score) to measure the resolvability of individual atoms, amino acid side chains, nucleotide bases, backbone atoms, water, ion and ligands in the cryoEM structures. We will demonstrate the usefulness of quantifying a cryoEM structure to describe its resolvability and accuracy in order to yield functional insights of the molecular complex.