MS10-P02 | ANALYSIS AND VALIDATION OF B VALUES OF MACROMOLECULAR STRUCTURES.

Masmaliyeva, Rafiga (ANAS Institute of Molecular Biology and Biotechnology, Baku, AZE); Murshudov, Garib (MRC Laboratory of Molecular Biology, Cambridge, GBR)

This presentation will describe a global analysis of macromolecular B values. It is shown that the distribution of B values generally follows the Shifted Inverse Gamma Distribution (SIGD). SIGD parameters are estimated using the Fisher scoring technique with the expected information matrix. It is demonstrated that a contour plot based on the parameters of SIGD can be used to validate macromolecular structures. The analysis of the dependence of the peak heights (PH) on resolution and atomic B values is shown. It is demonstrated that PH distribution depends on resolution and B values. A comparative analysis neighbouring atoms must account for resolution and B values. A combination of SIGD, PH distribution and outlier detection are used to identify entries from the PDB that require attention. It is also shown that presence of a multimodal B value distribution indicates that some parts of the molecule have been mismodelled or have different mobility, depending on their environment. These distributions can also indicate the level of sharpening/blurring of Fourier coefficients. Often sharpening/blurring is an artefact of data scaling, absolute average B value depends on the scaling technique used; the shape of B value distribution is invariant to scaling.

Sometimes atomic models exhibit multimodal B value distribution. In such cases, expectation maximisation method is used to model B value distributions as a mixture of SIGD.

Local analysis of B values and PH, a tool to identify mimodelled/misidentified atoms, will also be demonstrated.

Developed algorithms have been implemented in an open source software – ToBeValid.