MS10-P05 | B-FACTORS REFLECT THE LOCAL DYNAMICS OF PROTEINS AND NUCLEIC ACIDS

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Our recent analysis of scaled B factors in over 700 crystal structures of protein–DNA complexes showed that the B factor distributions of biopolymer residues, amino acids and nucleotides, as well as ordered water molecules, are a primary function of their neighborhood [1]. Amino acids in the interior of proteins have the tightest B factor distributions, residues forming the biopolymer interfaces have the distribution shifted to higher B factor values, and residues exposed to the solvent have the widest distribution with the mode at the highest B factor values. The distributions are also different for the backbone and side chain atoms and for the DNA backbone and base atoms. The behavior is evident in the group of structures with resolution higher than 1.9 Å and represents well the local protein and DNA dynamics. However, the distributions are much less telling at lower resolution bins and the factual meaning of B factors is lost. It stands to reason that residues in low resolution structures have principally similar local dynamics as residues in the high resolution structures. We therefore propose that the high resolution B factor distributions can be used to formulate the initial constraints for B factor values in structures refined at lower resolution.

[1] Schneider B et al. Acta Cryst. D70, 2413–2419 (2014). doi: 10.1107/S1399004714014631.