MS10-04 | Assessment of Model Bias in Crystallographic Maps and its Implications for Validation of Crystal Structures

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Since decades, model bias has been considered as the Achilles' heel of macromolecular crystallography due to the necessity of deriving the crystallographic phases from an atomic model and utilizing them for the calculation of an electron density map. As a consequence, the resulting map tends to possess features present in the atomic model regardless of their existence in the structure, in particular in cases when a partial model with errors has been used. The awareness of limitations caused by model bias, has led to the development of several methods aiming to reduce it: prime-and-switch phasing, composite omit map, ping-pong map, ‘kicked’ OMIT map, 'iterative-build' OMIT map, Feature-Enhanced Map (FEM), sigma-A weighting. Most of the mentioned methods address only one or a few map quality-related problems at a time and thus provide maps of different reliability and applicability for model re-building or validation. In order to assess both the quality and the level of model bias in commonly used crystallographic maps, a set of about 260 deposited crystal structures, for which a bias free SAD experimental electron density map of good quality could be obtained, has been analysed. Numerous map comparisons in both real and reciprocal space (the Fourier Shell Correlation, FSC) have been performed in an attempt to determine the least biased electron density map which should be the most suited for verification of structural model as well as for the subsequent validation. Application of the FSC for estimation of the quality of the crystal structure will be discussed.