Model dependence (IAM vs. TAAM) of B-factors cases of X-ray and electron diffraction

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It is known that B-factors correlate with measurement temperature, crystals quality, disorder, etc.. They also correlate with resolution. In case of X-ray diffraction (XRD) higher values of B-factors are connected with lower resolution [1]. In case of electron diffraction (3D-ED) there are additional factors: dynamic scattering and radiation damage, so the trend in B-factors values is not so obvious as for XRD. But is there a systematic difference between sizes of B-factors if the only variable is a model of static density? Would it be the same for different crystal structures (small organic molecules, polypeptides, proteins)? How would the difference depend on resolution? Would it be the same in case of X-ray and electron diffraction?

It was also shown, that different scattering models – e.g. Independent Atom Model (IAM; spherical, not describing bonds, lone pairs, charge transfer etc.) or Transferable Aspherical Atom Model (TAAM; describing asphericity, but in fixed manner, not refined) can be used for structure refinements with diffraction data [2]–[4]. Here we present comparison of B-factors from IAM and TAAM refinements of different types of crystal structures: carbamazepine (small molecule) from XRD and 3D-ED [5], [6], peptide pseudoxylallemycin A from XRD [7] and peptide OsPYL/RCAR5 from 3D-ED [8], lysozyme from XRD and 3D-ED [9], [10]. We observe systematic difference in B-factors from these two refinements, however, results still need discussion and we hoped for that during the poster sesion.

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