

Evaluating the Quality of MicroED Structures

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As a service provider of small molecule structure determination by MicroED, we have seen the gamut of high-quality structures with coordinates indistinguishable from scXRD to highly problematic structures with substantial disorder and/or those requiring significant restraints. Even the question of how to tell a problematic structure from a highly-quality structure is complicated by the generally higher R-factors produced by MicroED structures refined kinematically compared to those from scXRD. Not all MicroED structures with high R-factors are bad and relatively low R-factors don't always indicate a high-quality structure. In this short talk, I will present some of our recent structures and discuss how to think about the quality of MicroED structures and what conclusions can be drawn from them.