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Disordered Structures: Identification and Interpretation. Peter Y. Zavalij, Dept. of Chemistry and Biochemistry, Univ. of Maryland, MD 20742 USA.

Crystal structures often exhibit different kinds of disorder from simple and frequent solvent disorder and rotational disorder of terminal groups to quite rare whole molecule disorder and to complex micro-twinning and OD structures. Usually significant disorder can be easily identified by high R-factor, strange ellipsoids, or senseless difference peaks. However, sometimes disorder is not obvious and can be detected only by looking for some small, seemingly insignificant features, for example, difficulties in refinement of H atoms or presence of residual peaks even as small as hydrogen atom that are not near heavy atoms or in the middle of bonds, while the displacement ellipsoids are good and R-factor is just slightly higher than desired.

This presentation discusses identification and interpretation of the disordered structures covering several structures with whole molecule disorder, OD structure, an interesting stacking disorder in packing of 16! symmetrically independent molecules, and several structures of centrosymmetric host with non-centrosymmetric guest. The latter rises problem of choice between "classic" disordered structure and merohedral twinning: F vs. F². It was noticed that in many cases structure disorder happens in the presence of "unrealized" local symmetry of the molecules or other building blocks.