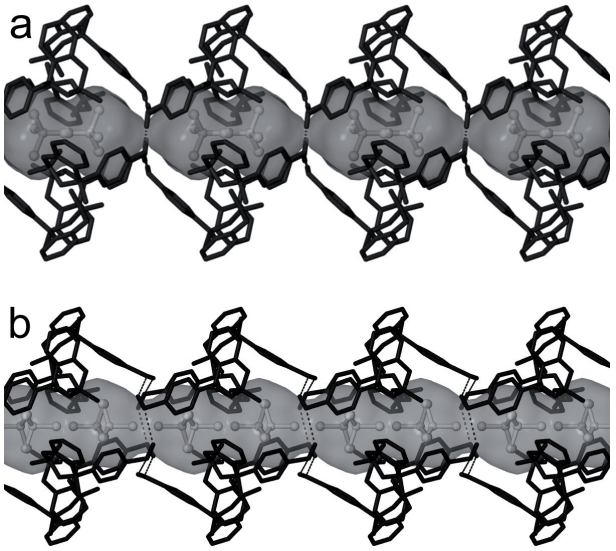
host frameworks may become porous if the guest molecules can be extracted without significant collapse of the host packing arrangement. When these processes occur as single-crystal to single-crystal transformations, it is possible to use crystallographic methods to establish structure-property relationships.

When multicomponent systems are able to include a range of different guest molecules within a predictable host framework, it is possible to tune properties by means of judicious choice of the guest. Examples involving polar ordering of guest molecules within well-defined host channels will be presented.



Keywords: inclusion compounds, porous materials, polar ordering

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Validation and errors in protein structures

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To err is human, and all macromolecular crystallographers are human - therefore, they are not immune to making errors during 3D model building and refinement [1]. Fortunately, many errors can be detected and fixed prior to publication and deposition by using common sense [1], appropriate protocols [2] and validation procedures [3].

In my lecture, I will discuss why errors are made and why some of them persist in published and deposited models, and hence why validation of 3D structure models is so important. I will describe what validation entails (both in general and for protein crystallography specifically) and explain why some validation criteria are more informative than others [4].

The Worldwide Protein Data Bank (wwPDB) recognises that validation is critically important for an archive of experimental structures and has therefore convened several Validation Task Forces or VTFs (for X-ray, NMR and EM). These VTFs are composed of community experts and have been asked to recommend procedures and criteria for the validation of models and data upon deposition in the PDB. The X-ray VTF has recently completed its report, and its recommendations are currently being implemented in a wwPDB validation pipeline. Its recommendations for model-only validation (e.g., geometry, torsion angles, clashes) will be adopted by the NMR and EM VTFs as well. The NMR VTF is expected to report its findings within the next year. Validation of EM maps and assessment of the fit between EM maps and models is still in its infancy and therefore the validation requirements for EM are anticipated to evolve slowly over the next 5 or so years. One important result of the work of all three VTFs is the identification of areas in which further research is required before consensus validation recommendations can be made. The use of comprehensive validation procedures will hopefully lead to fewer errors going undetected. Moreover, information about the quality of PDB and EMDB entries will be invaluable for structure users, many of whom are not experts in experimental structural biology [5]. However, challenges for the validation-research community remain, in particular in validating low-resolution models (X-ray, EM, SAXS) and hybrid models based on multiple heterogeneous sources of both experimental data and fitted models.

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Keywords: protein structure, validation, Protein Data Bank

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Prenucleation clusters and crystallization control by additives

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Prenucleation clusters are a stable species which was recently discovered for calciumcarbonate, -oxalate or –phosphate.[1] They already exist even in undersaturated solution, can have different solubilities / structures and were found to form amorphous nanoparticles by aggregation, which are the precursor structures for the final crystals. These clusters will be introduced and the driving force for their formation is discussed. If additives are added to a crystallization reaction, many parameters which characterize a nucleation reaction are influenced. Among them are supersaturation, nucleation inhibition / enhancement, change of the prenucleation cluster equilibrium, ion complexation and more. For several examples, it will be shown how the early stages of additive controlled crystallization can be quantitatively characterized and that additives usually play multiple roles in a crystallization reaction. The consequences of the different additive interactions for the final crystals will also be discussed.

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Keywords: nucleation, prenucleation clusters, crystallization additives