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A new space group determination algorithm is described that follows the structure solution step rather than preceeding it. It is based on an analysis of the average phase differences between symmetry equivalent reflections following the solution of the structure in space group P1. It is shown that this method performs very well for cases that are troublesome for space group determination algorithms based on an analysis of systematic extinct reflections. Examples illustrating the method include the analysis of weak data sets, faulty data sets, centrosymmetric/non-centrosymmetric ambiguity, ambiguous cases without systematic extinct reflections, data sets missing critical reflections, powder data and data from incommensurate crystal structures. The algorithm can be used as well for the analysis of missed higher symmetry.

Keywords: space group determination, structure solution, algorithm

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Tracing the protein main chain down to 5.5 Angstroms

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The crystals of many large protein assemblies diffract only to low resolution. To facilitate however their automatic structure determination a dedicated computational method has been developed that works with low resolution data down into the 5 Angstrom regime and even at very moderate phase quality. The method first recognises secondary structure elements and extends the main chain beyond these. It employs different tracing techniques to create an ensemble of candidate traces that are averaged to yield a solution in a robust way. The tracing techniques are supposed to introduce diversity into the ensemble in the way that they pick up noisy features at different places to different extent such that upon averaging this noise will to a good deal cancel out. For the ensemble average to be straightforwardly applicable a consensus between trace candidates is found with the help of clustering, trace alignment and majority voting. Typical positional errors of main chain CA atoms are not higher than of the order of 1 Angstrom. Through the use of sequence information and secondary structure prediction from sequence, restraints can be applied to the length of the main chain in between identified secondary structure elements as weights to ensemble participants. The software will be available as part of the ARP/wARP software suite whose version 7 as released in 2007 already contains the secondary structure modelling tool, a key component of the method proposed.

Keywords: structure determination, statistical analysis, low-resolution phasing

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SAXS, synchrotron CD and chemical cross-linking for structural study of complex biological systems

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Crystallography and NMR are unrivaled structural approaches for producing data-rich, atomic-resolution macromolecular structures though both suffer from stringent sample requirements. Furthermore, these techniques may not be the best approaches to use in cases where the biological questions relate to dynamics, transient interactions, non-stoichiometric complexes or flexible proteins. Various alternative structural biology approaches give different and complimentary information. Solution x-ray scattering can reveal the shape of a protein and the nature of quaternary interactions and dynamics. Circular dichroism reports on secondary structure and can be used dynamically. Chemical cross-linking with mass spectrometry can provide information on tertiary structure and protein-protein interfaces. Here I present the use of circular dichroism, small-angle x-ray scattering and cross-linking to study the structure of the filamentous actin binding protein cortactin and its effect on actin filaments. I also present the use of high-throughput synchrotron radiation circular dichroism and small-angle x-ray scattering to match uncharacterised proteins from a structural genomics project with protein of similar structure from the protein data bank.

Keywords: protein structure, small angle x-ray scattering, circular dichroism

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RAELS: A program for crystal structures that change across interfaces

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Two simple examples of structures changing across interfaces are twins and stacking faults. In the interface region the structure is different to the structure on either side of the interface. Crystals where this alternative structure extends for multiple layers are being observed but often ignored for the lack of a program that allows the coexistence of prototype structures and refinable rules for the creation of the observed diffraction patterns. Often the possibilities can be derived from an idealized, often disordered, parent structure of higher symmetry. Commensurability need not extend to three dimensions and may be approximate only, requiring lattice distortion at an interface. Chemical composition need not be the same for each prototype structure. Packing arguments can be used to show that many of these crystals should contain ordered layers but have different rules for relating adjacent layers. The asymmetric units for different prototype structures may be only approximately related by simple rules and comprehensive constraint and restraint options are then very useful. Crystals will vary in their population-type parameters and co-refinement of different crystals at the same temperature is useful. The author is completing his refinement program RAELS08 for the refinement of such structures and will discuss the comprehensive sets of options necessary for refining crystal structures that change across interfaces.

Keywords: refinement, twin-disorder, prototype structures