Our method employs *ab initio* polyalanine models (or 'decoys'), produced in large numbers then clustered based on the presence of similar core structures. The largest of these clusters is likely to be closest to the native structure [2]. Such *ab initio* modelling may result in an accurate prediction of the structural core of the target, but with inaccurate loops and termini. We have been developing an automated pipeline for the processing of *ab initio* models for use in Molecular Replacement. We show that truncation and clustering of models into ensembles can give a successful result where a single search model would fail. We find that the addition of a selection of side chains can also be used to improve the success rate.

Importantly, the likely success or failure of the modelling can be predicted based on characteristics of the protein such as length and secondary structure, and by the convergence of the modelling program to produce a large cluster of models with a similar core structure. Predictions of success can be given at each stage of the pipeline as data are accumulated to give feedback to the user, and to prioritise models for use in Molecular Replacement.

The pipeline has been tested on 241 proteins between 40-120 residues long, using Rosetta to produce 1000 decoys for each target. Ensembles were produced from these decoys, and Molecular Replacement carried out using MrBUMP. For 40 proteins, at least one search model was placed within 3Å of the deposited structure by MrBUMP, and in a further 42 cases, one or more search model was positioned to within 3-6Å. In 137 cases, ARP/wARP rebuilds resulted in mapping of traced residues to sequence. Of these, 71 proteins show a 50% or greater sequence coverage ratio with 20% or more of the backbone traced.

We have thus shown that *ab initio* modelling can be a viable route to structure solution for many small proteins. Initial results with other *ab initio* programs show success where Rosetta models failed. Similarly, we are extending this work to other rebuilding programs such as buccaneer which may well improve performance further.

This pipeline will be made freely available, and may ultimately require only the input of the protein sequence along with the experimental data. Unlike other computationally intensive methods [3], this method is suitable for modest hardware, allowing for broader adoption.

[1] R. Das, D. Baker, *Acta Crystallogr D Biol Crystallogr*. **2009**, *65*, 169-175.
[2] D.J. Rigden, R.M. Keegan, M.D. Winn, *Acta Cryst*. **2008**, *D64*, 1288-1291.
[3] B. Qian, S. Raman, R. Das, P. Bradley, A.J. McCoy, R.J. Read, D. Baker *Nature* **2007**, *450*, 259-264.

Keywords: modelling, molecular_replacement, automated_ structure_solution

MS.58.5

Acta Cryst. (2011) A**67,** C135

Release 7.2 of ARP/wARP software suite

Saul Hazledine,[a] Gerrit Langer,[a] Tim Wiegels,[a] Ciaran Carolan,[a] Philipp Heuser,[a] Krista Joosten,[b] Anastassis Perrakis,[b] Victor Lamzin,[a] [a]*European Molecular Biology Laboratory, Hamburg, (Germany).* [b]*The Netherlands Cancer Institute, Amsterdam, (The Netherlands).* E-mail: s.hazledine@embl-hamburg.de

ARP/wARP is a software project for automated model building and refinement in macromolecular crystallography. The software is the result of years of development in the areas of X-ray crystallography, informatics and statistical pattern recognition. ARP/wARP is an iterative procedure based on the use of hybrid macromolecular models that is integrated with model refinement and reconstruction to provide a unified approach. The software protocols are computationally efficient and provide an easy-to-use pipeline for the building of models of proteins, poly-nucleotides, bound ligands and solvent.

Version 7.2 of ARP/wARP was recently released and contains new techniques and approaches for the building models of large, low-resolution structures using non-crystallographic symmetry (NCS) and motif searching. NCS-related parts of a structure are rarely built in the same way during model building. A beneficial side effect of this is that each copy provides information that is not present in another copy. By combining this intrinsic information the model building process is improved and the overall completeness of built structures at low resolution is increased. Coupled with novel implementations for enhanced protein chain tracing, the use of NCS provides improvements of up to 18% in model completeness (from 55% to 73% at 3.2Å, for example).

Further developments include automation in modelling of bound ligands that are partially ordered. The electron density map can be automatically screened for density corresponding to any of a cocktail of potential ligands and those that fit best are automatically built. Furthermore, in instances where the density is insufficient to allow accurate identification of atomic coordinates of particular ligands, 'partial' ligands, comprised only of the fragments whose atoms are in unequivocal density, can be modelled.

The graphical front-end *Arpnavigator* allows users to view models in real time while they are automatically built and refined. With the 7.2 release the functionality of the front-end has been considerably extended, and new file formats and display styles of molecules are supported. Publication quality images in standard colours are now easier to produce.

Keywords: model_building, refinement, crystallographic_ Software

MS.59.1

Acta Cryst. (2011) A**67,** C135-C136

Halogen vs. Hydrogen bonding in the design of anion receptors

Pierangelo Metrangolo,[a,b] Serena Biella,[a,b] Gabriella Cavallo,[b] Tullio Pilati,[a] Giuseppe Resnati,[a,b] Giancarlo Terraneo,[a,b] [a]*NFMLab, DCMIC "Giulio Natta", Politecnico di Milano, Milano (Italy).* [b]*CNST-IIT, Politecnico di Milano, Milano (Italy).* E-mail: pierangelo.metrangolo@polimi.it

Halogen bonding (XB), namely any noncovalent interactions involving the positive region of the electrostatic potential surface of halogen atoms [1], has proven its efficiency and reliability in supramolecular chemistry, crystal engineering, and materials science [2]. Its potential and use in anion coordination and anion-templated assembly has been discovered and investigated only recently [3].

In this contribution, we report some examples of anion binding driven by halogen bonding where halides anions act as halogen bonding acceptors.

We will also present how XB directs the self-assembly of oxyanions, by far the most numerous class of anions in organic chemistry, forming discrete adducts and 1D, 2D, or 3D supramolecular networks with halocarbons. Some specific examples will be discussed in order to identify new supramolecular synthons based on halogen bonding and to outline some general principles for the design of effective and selective receptors based on this interaction [4].

It will be demonstrated that the replacement of hydrogen with halogen atoms into anion receptor scaffolds may develop as a convenient strategy to improve binding and selectivity.