structural folds in the frame of ARCIMBOLDO_SHREDDER will be illustrated.

References:

[1]. Williams, C. J. et al. (2018) Protein Science 27:293-315
[2]. Sammito, M et al. (2013) Nature Methods 10:1099–1101
[3]. Millán, C et al. (2015) IUCrJ 2:95-105

Keywords: secondary structure annotation, geometry, phasing

MS12-P02

Overcoming phasing difficulties in coiled-coils with ARCIMBOLDO_LITE: verifying solutions

Iracema Caballero Muñoz[1], Massimo Sammito [1], Claudia Millán[1], Nicolas Soler[1], Andrey Lebedev[2], Isabel Usón[1]

1. Structural Biology Unit, Institute of Molecular Biology of Barcelona (IBMB–CSIC), Barcelona, Spain
2. CCP4, STFC Rutherford Appleton Laboratory, Research Complex at Harwell, Oxford, Great Britain

email: icmcri@ibmb.csic.es

ARCIMBOLDO_LITE is an *ab initio* phasing approach that combines location of small, very accurate model fragments with PHASER followed by density modification and main chain autotracing with SHELXE. Mainly helical structures are favorable cases for this approach, as ideal polyalanine α-helices constitute an excellent approximation of helices in real structures. Coiled coil structures, despite being highly helical, typically present intrinsic difficulties for phasing.

In general, for all coiled coils structures, it can be complicated to distinguish whether prominent features in the Patterson function are due to genuine tNCS or to the intrinsic periodicity of the helix. In addition, often mistranslated solutions reach high scores. This can lead to elimination of all starting hypotheses through the packing filters. At low resolution (2-3Å), the placement of helices occasionally takes place in the correct position but in reversed direction. Also, even when having a correct substructure placed, autotracing the helices from a very partial solution in a map degraded by severe anisotropy, modulation and limited resolution is challenging. And finally, after tracing, the discrimination of correct from the incorrect solutions can be misleading, requiring a final verification step. To overcome these difficulties ARCIMBOLDO_LITE [1] incorporates a set of improvements gathered under a specific *coiled_coil* mode, exploiting new improvements in PHASER [2] and SHELXE [3].

These features were designed for solving coiled coils at resolutions up to 3Å and tested on a pool of 150 structures, showing a 93% success rate. Furthermore, this implementation has allowed to solve new previously unknown structures, and unequivocally identifies correct solutions through the new verification strategy. This idea opens promising perspectives to extend its application within the use of small general model fragments.

References:

[1] Caballero, I., Sammito, M., Millan, C., Lebedev, A., Soler, N. & Uson, I. (2018). Acta Cryst. D74, 194-204.
[2] Oeffner, R. D., Afonine, P., Millán, C., Sammito, M., Usón, I., Read, R. J. & McCoy, A. J. (2018). Acta Cryst. D74. In the press.
[3] Usón, I. & Sheldrick, G. M. (2018). Acta Cryst. D74, 106–116.

Keywords: ARCIMBOLDO, coiled coils, phasing