MS21-1-3 Towards understanding of structure modulation in macromolecular system of Hyp-1/ANS protein complex
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Abstract
The phenomenon of crystal structure modulation is quite widespread and well-understood in small-molecule crystallography, but in macromolecular crystallography is almost unheard of [1]. Modulated structures are characterized by the disappearance of short-range translational order restored in long-range by an atomic modulation function (AMF). Rigorous analysis of incommensurate modulation requires interpretation of diffraction pattern as a three dimensional projection of a higher dimensional reciprocal lattice [2]. Existing, routinely used procedures for solving and refinement of protein structures are not suitable for complex analysis of modulated structures. In cases of incommensurate modulation even the data processing might be an insurmountable problem. Our research include analysis of Hyp-1/ANS protein complexes using a higher-dimensional approach with modulation vector implemented as another dimension. Any assumptions of commensurateness were rejected and special corrections for twinning, pseudosymmetry and structural disorder such as phonons were introduced to improve structure model and reduce high R factors values. Deviation of atom position relative to its average position in three-dimensional space can be reconstructed by shape of the AMF. As a model structures, unique Hyp-1/ANS modulated protein complexes were chosen [1,3]. The re-integration of raw data was performed in CrysAlisPro software with detailed analysis of weak satellite reflections, while phase problem was resolved using Superflip – software based on charge flipping algorithm. For structure modelling and refinement, original software written in Matlab environment with introduced corrections for structural disorder was used. Optimization method used during refinement based on metaheuristics and genetic algorithms against traditional maximum likelihood targets. Therefore, new software dedicated to structure analysis of modulated macromolecular systems will be shared to other users.

References
[1] Sliwiak, J., Dauter, Z., McCoy, A., Jaskolski, M. & Read, R.J. (2014). Acta Cryst. D70, 471-480.
[2] Wolny, J., Buganski, I., Kuczera, P. & Strzalka, R. (2016). J. Appl. Crystallogr. 49, 2106-2115.
[3] Sliwiak, J., Dauter, Z., Kowiel, M., McCoy, A., Read, R.J & Jaskolski, M. (2015). Acta Cryst. D71, 829-843.