High Symmetry Involved in Cellular Regulation

Dominika Borek, Yuanhong Chen, Mingzhu Zheng, Zbyszek Otwinowski, *Department of Biochemistry, UT Southwestern Medical Center at Dallas.* E-mail: dominika@work.swmed.edu

170aa protein product of Ycfc gene crystallized in space group P23 with unit cell axes of 230.6 Å. The expected numbers of methionines in the A.U. (~240) discouraged Se-Met approach. SIRAS data for the Hg-derivative were collected to 4.2 Å. However, NCS could not been identified by standard programs. Derivative crystals had a substantial non-isomorphism with native data. Moreover, native Patterson map indicated translational pseudosymmetry. NCS was found using *ad hoc* software based on guessing the NCS arrangement from space group and packing considerations. The structure was solved by a combination of SAD phasing, NCS averaging and multiple crystal averaging.

Structural analysis revealed 2 identical, 24-meric oligomeric assemblies with 432 symmetry, placed on a diagonal, 3-fold crystallographic axis. At every non-crystallographic four-fold axis two molecules of Cl^- ligand were identified.

Based on crystallographic and sequence conservation analysis, we hypothesize that this complex regulates gene activity, with Cl ions stabilizing a highly symmetrical form, possibly active as a repressor and/or activator of transcription. Binding of 12 Cl ions in a symmetrical assembly potentially creates a very steep response to chloride ion concentration.

Crystallographic and biophysical data will be presented for potential regulation mechanism.

Keywords: non-crystallographic symmetry, pseudosymmetry, regulation