## MS12-P03 | SYMMETRY IN STRUCTURES OF PROTEIN ASSEMBLIES

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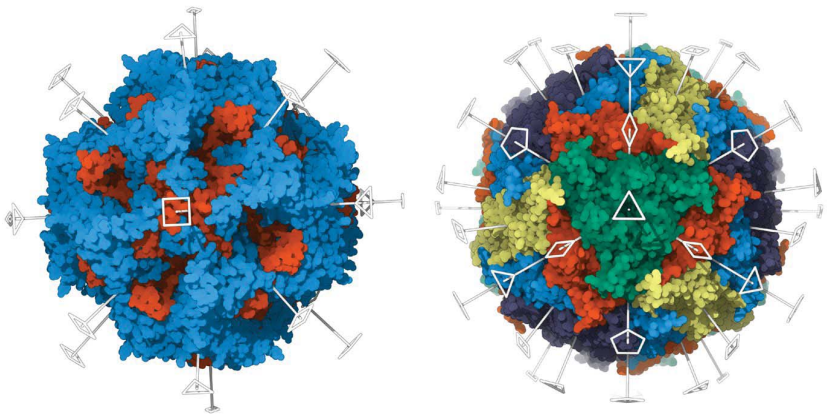

Many protein complexes in the Protein Data Bank (PDB) are symmetric homo-oligomers. Indeed, it appears that large symmetrical protein structures have evolved in many organisms because they carry specific morphological and functional advantages compared to small individual protein molecules. There is therefore considerable interest in studying and modelling these assemblies.

Recently we have proposed a novel free-docking method for protein complexes with arbitrary point-group symmetry [1]. It assembles complexes with cyclic symmetry, dihedral symmetry, and also those of high order (tetrahedral, octahedral, and icosahedral). Later on we discovered that the inverse problem, i.e. identification of symmetry in a protein assembly, is even more interesting. Given a structure of the assembly, it consists in the identification of the symmetry measure, and also of the computations of the symmetry axes [2-4]. We tackled this problem using two orthogonal approaches, (i) analytical minimization of a geometrical mismatch score over transformation operators within a symmetry group [2-3]; and (ii) convolutional neural networks trained on 3D density maps [4]. Using these tools, we performed exhaustive analysis of all symmetric structures in the PDB and found some organization patterns that are worth discussing.

[1] Ritchie, D. W. & Grudinin, S (2016). *J. Appl. Cryst.*, **49**, 1-10.
{2] Pages, G., Kinzina, E, & Grudinin, S (2018). *J. Struct.Biology*, **203** (2), 142-148.
[3] Pages, G. & Grudinin, S (2018). *J. Struct.Biology*, **203** (3), 185-194.
[4] Pages, G. & Grudinin, S (2018). *arXiv preprint* arXiv:1810.12026.