IHM Meeting

May 24th, 2018

Agenda

- Update on the IHM-dictionary and PDB-Dev
- Update on the Python-IHM library
- Open discussion

PDB-Dev

- 15 structures have been released
  - Software: IMP, Rosetta, HADDOCK, TADbit, XPLOR-NIH
  - Restraints: NMR, CX-MS, 2DEM, 3DEM, SAS, FRET, Predicted Contacts from high-throughput sequencing, Hi-C, Mutagenesis, DNA Footprinting
- 2 are on hold for publication
  - EPR
- Other structures under process
  - Rosetta, FRET-based modeling using FPS software
- NPC structure published in Nature has PDB-Dev accession codes
  - Kim SJ, Fernandez-Martinez J, Nudelman I, Shi Y, et al., Nature. 2018 Mar; 555(7697):475-82
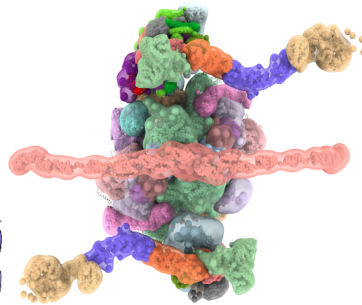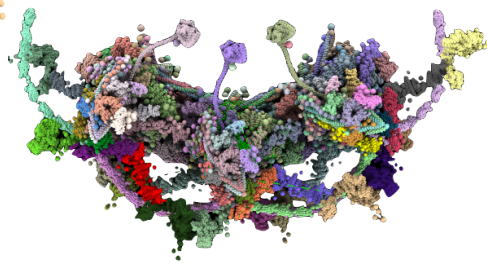
Structures in PDB-Dev

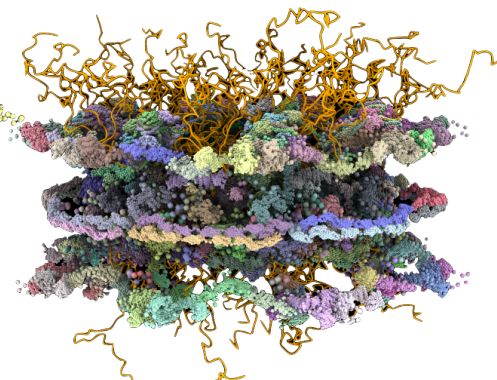Nup 84
PDBDEV_00
000001
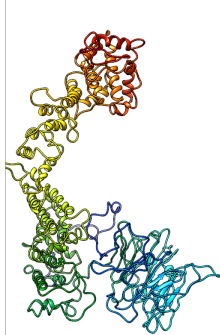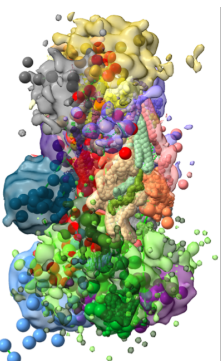
Nup 133
PDBDEV_00
000016

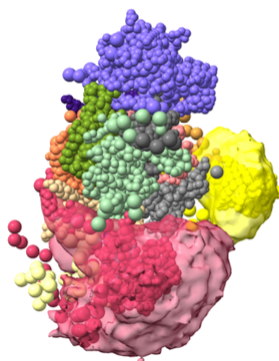Pom 152
PDBDEV_00
000017

NPC 1 spoke
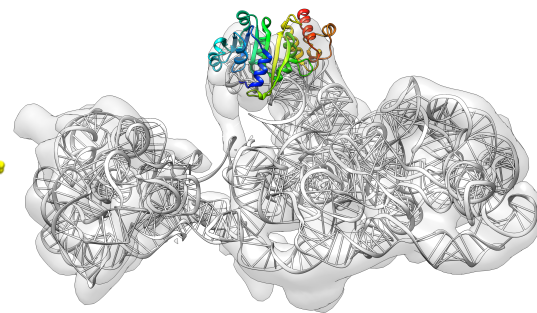PDBDEV_
00000010

NPC 3 spokes
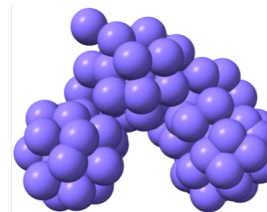PDBDEV_00000011

NPC 8 spokes
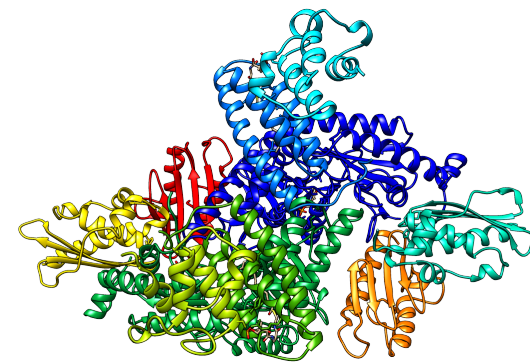PDBDEV_00000012

Mediator
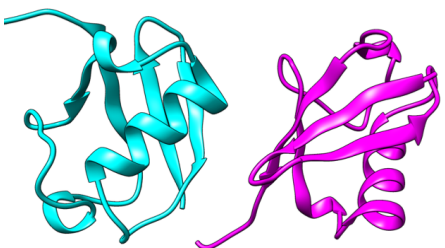PDBDEV_00
000003

Exosome
PDBDEV_00
000002

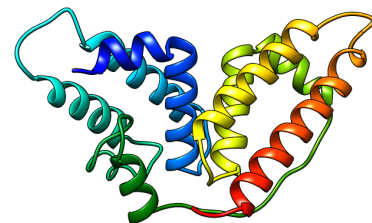16s RNA – Methyltransferase A
PDBDEV_00000014

Fruit fly Chromosome 2L
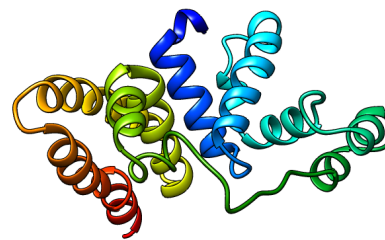segment
PDBDEV_00000008

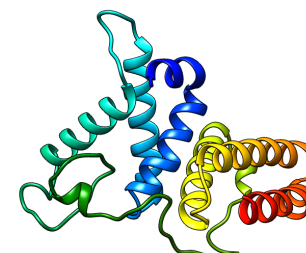Mitochondrial Cysteine desulfurase
PDBDEV_00000015

Diubiquitin
PDBDEV_00000004

Human Serum Albumin Domain A
PDBDEV_00000005

Human Serum Albumin Domain B
PDBDEV_00000006

Human Serum Albumin Domain C
PDBDEV_00000007

IHM-dictionary updates

- Added a categories for generic distance restraints
    - HADDOCK Ambiguous Interaction Restraints (AIR)
    - Restraints from EPR experiments

- Restraints to geometric objects
    - Membrane represented as a half-torus in NPC modeling

- Ongoing process as we get more examples spanning different kinds of experiments

- Paper accepted for publication in Structure
    - Vallat B, Webb B, Westbrook JD, Sali A, Berman HM. Development of a Prototype System for Archiving Integrative/Hybrid Structure Models of Biological Macromolecules. Structure. 2018. doi: 10.1016/j.str.2018.03.011.

Python-IHM library

- https://github.com/ihmwg/python-ihm

Open Discussion