

# Support of IHM mmCIF format in HADDOCK 2.4

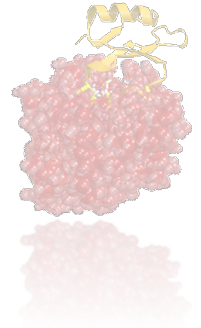
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111000100101010110101010
100011010101000101111010110101
10100001000111101010101110000110101
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# Objectives



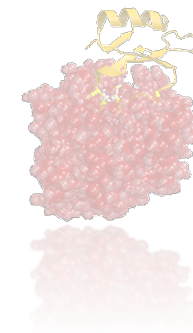
- **IHM PDBx/mmCIF files accepted as input...**
  - ✓ Read/convert atom\_site information (coordinates, segid, etc.)
  - ☰ Read/convert experimental data as parameters (EM map, Xlinks, etc.)
- **... and output - generation of IHM PDBx/mmCIF from the results page**
  - ✓ Generate atom coordinates only
  - ☰ Generate atom coordinates + interface (ihm\_model\_representation)
  - ☰ Generate atom coordinates + interface + restraints

1) Single model

2) Ensemble of models (cluster)
- **Use mmCIF as internal format for pre- and post-processing**
  - 💬 Feasibility to be discussed, involves significant efforts



# Conclusion



- Different read/write modules rely on python-ihm (<https://github.com/ihmwg/python-ihm>)
- Preview of beta-version:

**Summary**

HADDOCK clustered **11** structures in **6** cluster(s), which represents **55 %** of the water-refined models HADDOCK generated. Note that currently the maximum number of models considered for clustering is **100**.

**WARNING:** Clustering with default parameters did not produce any cluster, cluster minimum size went from **4** to **3**


The statistics of the top 10 clusters are shown below. The top cluster is the most reliable according to HADDOCK. Its Z-score indicates how many standard deviations from the average this cluster is.

A graphical representation of the results is also provided at the bottom of the page.

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**CLUSTER 1**

|   |                 |
|---|-----------------|
| HADDOCK score                                 | -8654.5 +/- 7.5 |
| Cluster size                                  | 3               |
| RMSD from the overall lowest-energy structure | 0.6 +/- 0.4     |
| Van der Waals energy                          | -43.8 +/- 4.7   |
| Electrostatic energy                          | -216.1 +/- 8.8  |
| Desolvation energy                            | -13.1 +/- 2.6   |
| Restraints violation energy                   | 0.0 +/- 0.0     |
| Buried Surface Area                           | 1555.7 +/- 52.9 |
| Z-Score                                       | -1.7            |

Nr 1 best structure [Download file](#) 

Nr 2 best structure [Download file](#)

Nr 3 best structure [Download file](#)

**CLUSTER 5**

|   |                 |
|---|-----------------|
| HADDOCK score                                 | -1090.9 +/- 0.1 |
| Cluster size                                  | 5               |
| RMSD from the overall lowest-energy structure | 10.9 +/- 0.1    |
| Van der Waals energy                          | -31.7 +/- 0.5   |
| Electrostatic energy                          | -90.8 +/- 40.0  |

[PDB Format](#)

[PDBx/mmCIF Format \(atom only\)](#)

[PDBx/mmCIF Format \(atom + interface info\)](#)

[PDBx/mmCIF Format \(atom + interface + restraints\)](#)

