HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-10"

Status: FINISHED

Your HADDOCK run has successfully completed. The complete run can be downloaded as a gzipped tar file **here**.
The file containing your docking parameters is **here**.

Please cite the following paper in your work:

G.C.P van Zundert, J.P.G.L.M. Rodrigues, M. Trellet, C. Schmitz, P.L. Kastritis, E. Karaca, A.S.J. Melquiond, M. van Dijk, S.J. de Vries and A.M.J.J. Bonvin (2016). "The HADDOCK2.2 webserver: User-friendly integrative modeling of biomolecular complexes."
J. Mol. Biol., **428**, 720-725 (2015).

and add the following acknowledgment:

The FP7 WeNMR (project# 261572), H2020 West-Life (project# 675858), the EOSC-hub (project# 777536) and the EGI-ACE (project# 101017567) European e-Infrastructure projects are acknowledged for the use of their web portals, which make use of the EGI infrastructure with the dedicated support of CESNET-MCC, INFN-PADOVA-STACK, INFN-LNL-2, NCG-INGRID-PT, TW-NCHC, CESGA, IFCA-LCG2, UA-BITP, SURFsara and NIKHEF, and the additional support of the national GRID Initiatives of Belgium, France, Italy, Germany, the Netherlands, Poland, Portugal, Spain, UK, Taiwan and the US Open Science Grid.

How would you rate your experience with our portal?

Questions / feedback ? ask.bioexcel.eu

Do check up the HADDOCK best practice guide! There you can learn more about which settings are best used in which scenario and use HADDOCK in its full potential!

In the aim to improve our new web portal, we would really appreciate 2 min of your time to complete a short survey here! Thanks!

Post-processing: SUCCESS

Summary

HADDOCK clustered **190** structures in **10** cluster(s), which represents **95 %** of the water-refined models HADDOCK generated. Note that currently the maximum number of models considered for clustering is 200.

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 located in terms of score (the more negative the better).

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

You can also download all cluster files (best 4 of the top 10 cluster(s)).

Cluster 2

HADDOCK score	-79.6 +/- 0.7
Cluster size	51
RMSD from the overall lowest-energy structure	5.6 +/- 0.4
Van der Waals energy	-57.6 +/- 4.0
Electrostatic energy	-225.2 +/- 21.9
Desolvation energy	-7.6 +/- 1.7
Restraints violation energy	306.2 +/- 30.7
Buried Surface Area	1819.9 +/- 64.4
Z-Score	-1.4

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 1

HADDOCK score	-79.2 +/- 2.1
Cluster size	56
RMSD from the overall lowest-energy structure	18.2 +/- 1.3
Van der Waals energy	-62.8 +/- 6.3
Electrostatic energy	-186.1 +/- 11.5
Desolvation energy	-6.3 +/- 2.6
Restraints violation energy	271.1 +/- 53.1
Buried Surface Area	1852.4 +/- 48.5
Z-Score	-1.4

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 4

HADDOCK score	-72.4 +/- 8.3
Cluster size	16
RMSD from the overall lowest-energy structure	0.6 +/- 0.4
Van der Waals energy	-62.5 +/- 4.4
Electrostatic energy	-111.2 +/- 18.0
Desolvation energy	-11.1 +/- 4.9
Restraints violation energy	235.5 +/- 61.0
Buried Surface Area	1857.0 +/- 55.3

Z-Score	-0.5

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 7

HADDOCK score	-72.2 +/- 1.5
Cluster size	8
RMSD from the overall lowest-energy structure	12.4 +/- 0.3
Van der Waals energy	-58.9 +/- 4.8
Electrostatic energy	-170.6 +/- 27.1
Desolvation energy	-7.2 +/- 4.6
Restraints violation energy	280.8 +/- 33.8
Buried Surface Area	1902.7 +/- 88.3
Z-Score	-0.5

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 9

HADDOCK score	-71.2 +/- 7.7
Cluster size	4
RMSD from the overall lowest-energy structure	21.5 +/- 0.2
Van der Waals energy	-59.3 +/- 4.9
Electrostatic energy	-202.2 +/- 16.8
Desolvation energy	0.1 +/- 1.0
Restraints violation energy	284.7 +/- 8.6
Buried Surface Area	1962.9 +/- 89.0
Z-Score	-0.4

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 6

HADDOCK score	-65.5 +/- 6.1

Cluster size	9
RMSD from the overall lowest-energy structure	14.9 +/- 0.3
Van der Waals energy	-54.3 +/- 4.5
Electrostatic energy	-150.6 +/- 15.4
Desolvation energy	-5.4 +/- 4.2
Restraints violation energy	242.8 +/- 47.9
Buried Surface Area	1936.1 +/- 37.8
Z-Score	0.4

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 5

HADDOCK score	-64.8 +/- 5.5
Cluster size	10
RMSD from the overall lowest-energy structure	23.0 +/- 0.2
Van der Waals energy	-48.8 +/- 2.6
Electrostatic energy	-136.3 +/- 32.2
Desolvation energy	-9.5 +/- 1.6
Restraints violation energy	208.2 +/- 67.9
Buried Surface Area	1551.3 +/- 74.3
Z-Score	0.5

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 3

HADDOCK score	-63.4 +/- 3.9
Cluster size	26
RMSD from the overall lowest-energy structure	13.1 +/- 0.3
Van der Waals energy	-51.8 +/- 6.5
Electrostatic energy	-149.6 +/- 57.9
Desolvation energy	-6.6 +/- 3.4
Restraints violation energy	248.3 +/- 7.6
Buried Surface Area	1555.2 +/- 126.3
Z-Score	0.6

Nr 1 best structure Download file

Nr 2 best structure Download file

Nr 3 best structure Download file

Nr 4 best structure Download file

Cluster 10

HADDOCK score	-62.7 +/- 7.2
Cluster size	4
RMSD from the overall lowest-energy structure	17.5 +/- 1.0
Van der Waals energy	-65.8 +/- 5.8
Electrostatic energy	-78.8 +/- 13.2
Desolvation energy	-8.3 +/- 1.5
Restraints violation energy	271.5 +/- 38.8
Buried Surface Area	1848.2 +/- 143.6
Z-Score	0.7

Nr 1 best structure Download file

Nr 2 best structure Download file

Nr 3 best structure Download file

Nr 4 best structure Download file

Cluster 8

HADDOCK score	-52.7 +/- 8.3
Cluster size	6
RMSD from the overall lowest-energy structure	21.2 +/- 0.2
Van der Waals energy	-50.6 +/- 5.8
Electrostatic energy	-111.5 +/- 21.2
Desolvation energy	-13.3 +/- 3.3
Restraints violation energy	335.3 +/- 122.1
Buried Surface Area	1373.0 +/- 51.3
Z-Score	2.0

Nr 1 best structure Download file

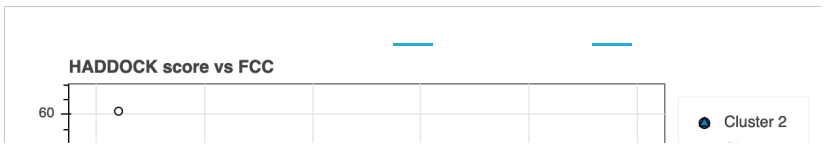
Nr 2 best structure Download file

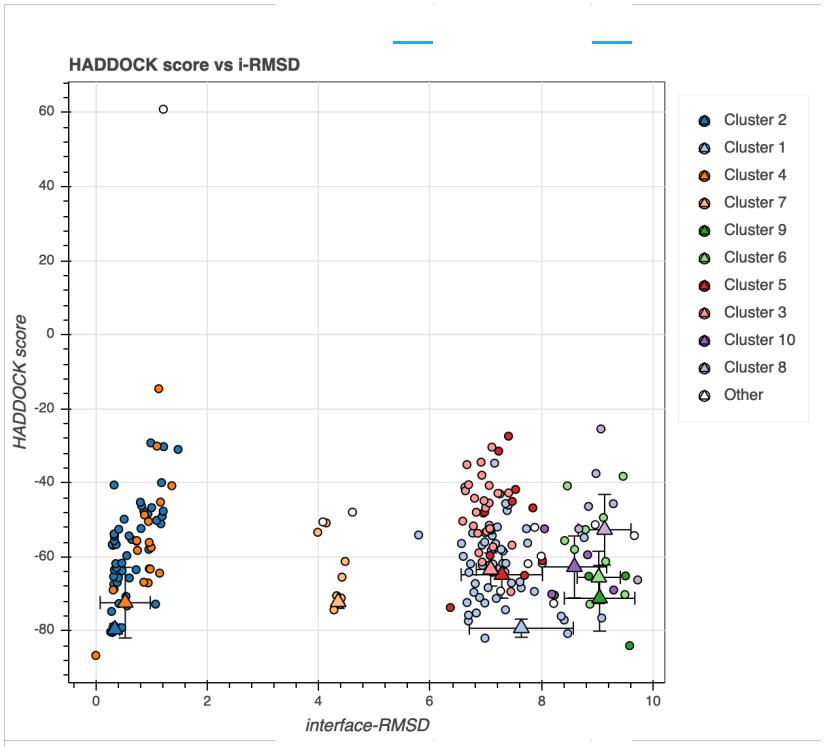
Nr 3 best structure Download file

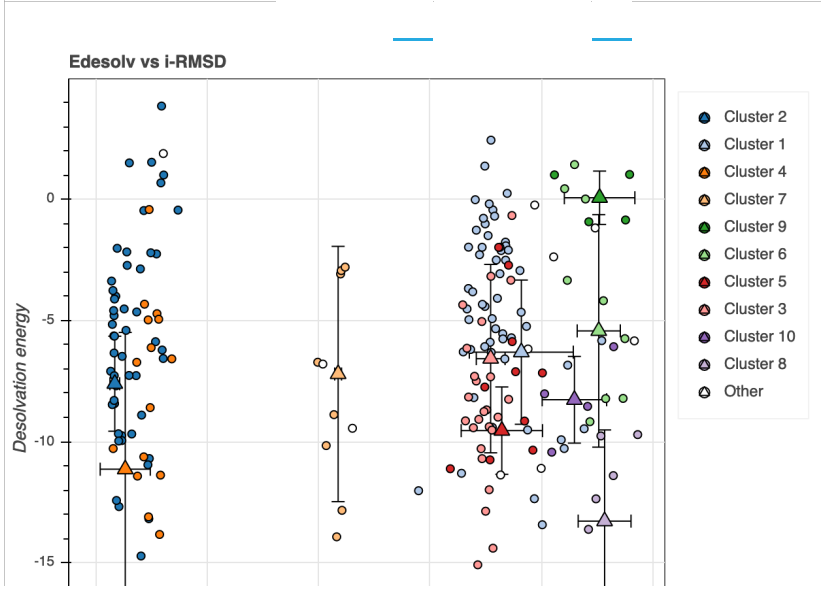
Nr 4 best structure Download file

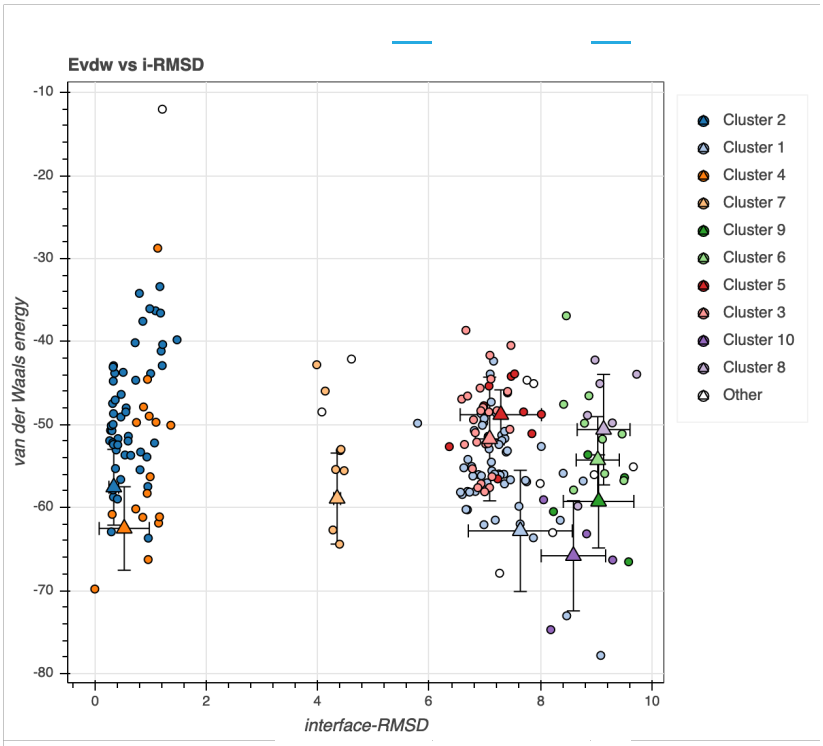
Model Analysis (Download all plots)

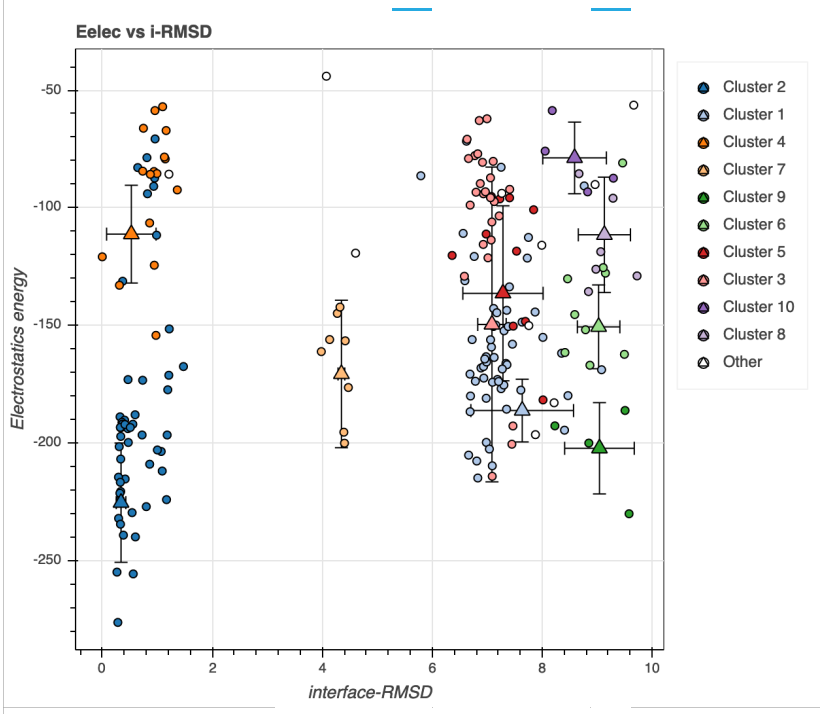
All | None | Cluster 2 | Cluster 1 | Cluster 4 | Cluster 7 | Cluster 9 | Cluster 6 | Cluster 5 | Cluster 3 | Cluster 10 | Cluster 8 | C

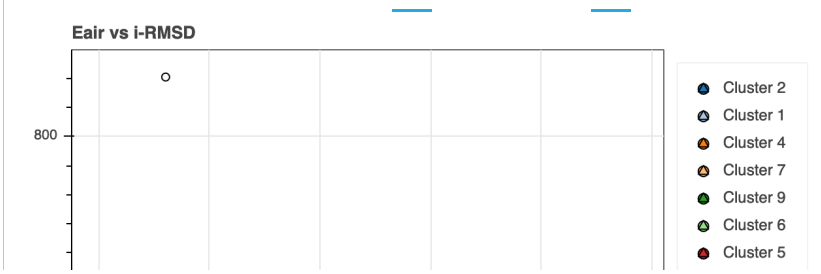



HADDOCK score vs i-RMSD
HADDOCK score
interface-RMSD
60
40
20
0
-20
-40
-60
-80
0
2
4
6
8
10
Cluster 2
Cluster 1
Cluster 4
Cluster 7
Cluster 9
Cluster 6
Cluster 5
Cluster 3
Cluster 10
Cluster 8
Other


Edesolv vs i-RMSD
Desolvation energy
0
-5
-10
-15
Cluster 2
Cluster 1
Cluster 4
Cluster 7
Cluster 9
Cluster 6
Cluster 5
Cluster 3
Cluster 10
Cluster 8
Other

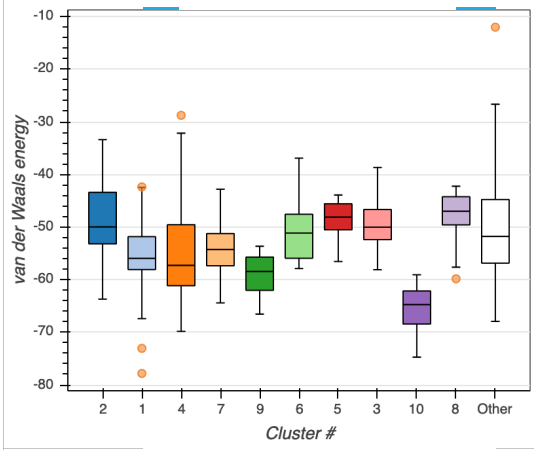

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
-10
-20
-30
-40
-50
-60
-70
-80
0
2
4
6
8
10
Cluster 2
Cluster 1
Cluster 4
Cluster 7
Cluster 9
Cluster 6
Cluster 5
Cluster 3
Cluster 10
Cluster 8
Other

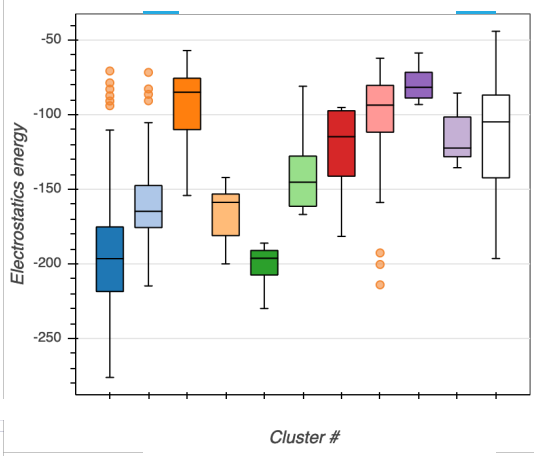

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
-50
-100
-150
-200
-250
0
2
4
6
8
10
Cluster 2
Cluster 1
Cluster 4
Cluster 7
Cluster 9
Cluster 6
Cluster 5
Cluster 3
Cluster 10
Cluster 8
Other

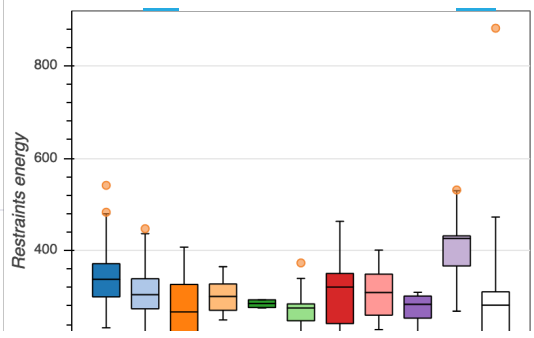

Eair vs i-RMSD
800
Cluster 2
Cluster 1
Cluster 4
Cluster 7
Cluster 9
Cluster 6
Cluster 5

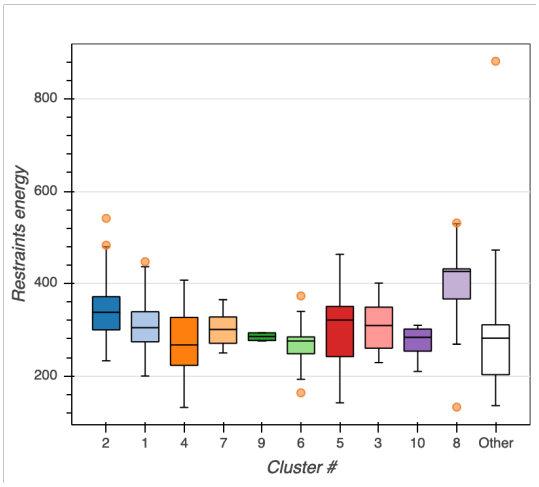
Cluster Analysis

All | None | Cluster 2 | Cluster 1 | Cluster 4 | Cluster 7 | Cluster 9 | Cluster 6 | Cluster 5 | Cluster 3 | Cluster 10 | Cluster 8 | C








Restraints energy
800
600
400
200
2
1
4
7
9
6
5
3
10
8
Other
Cluster #