

HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-32"

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. Kastiris, E. Karaca, A.S.J. Melquiand, 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 **177** structures in **6** cluster(s), which represents **88 %** 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 1

HADDOCK score	-101.8 +/- 2.4
Cluster size	76
RMSD from the overall lowest-energy structure	6.9 +/- 0.9
Van der Waals energy	-75.9 +/- 4.7
Electrostatic energy	-178.2 +/- 32.9
Desolvation energy	-14.0 +/- 3.4
Restraints violation energy	237.8 +/- 50.9
Buried Surface Area	2076.5 +/- 68.5
Z-Score	-1.2

Nr 1 best structure

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Nr 2 best structure

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Nr 3 best structure

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Nr 4 best structure

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Cluster 3

HADDOCK score	-93.7 +/- 1.7
Cluster size	18
RMSD from the overall lowest-energy structure	13.9 +/- 0.1
Van der Waals energy	-77.2 +/- 2.4
Electrostatic energy	-170.2 +/- 15.4
Desolvation energy	-8.0 +/- 1.3
Restraints violation energy	255.4 +/- 26.0
Buried Surface Area	1914.7 +/- 41.1
Z-Score	-0.5

Nr 1 best structure

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Nr 2 best structure

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Nr 3 best structure

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Nr 4 best structure


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Cluster 5


HADDOCK score	-93.4 +/- 12.1
Cluster size	8
RMSD from the overall lowest-energy structure	0.6 +/- 0.6
Van der Waals energy	-73.0 +/- 7.9
Electrostatic energy	-152.2 +/- 17.8
Desolvation energy	-12.5 +/- 3.7
Restraints violation energy	224.9 +/- 33.6
Buried Surface Area	2135.8 +/- 131.9


Z-Score -0.5

- Nr 1 best structure




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- Nr 2 best structure



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- Nr 3 best structure



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- Nr 4 best structure



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Cluster 4

HADDOCK score -87.0 +/- 6.5

Cluster size 9

RMSD from the overall lowest-energy structure 17.1 +/- 0.1

Van der Waals energy -68.9 +/- 2.9

Electrostatic energy -211.3 +/- 23.1


Desolvation energy -6.9 +/- 2.2

Restraints violation energy 309.5 +/- 53.5

Buried Surface Area 2021.0 +/- 30.0

Z-Score 0.0

- Nr 1 best structure




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- Nr 2 best structure



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- Nr 3 best structure



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- Nr 4 best structure



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Cluster 2

HADDOCK score -85.9 +/- 8.7

Cluster size 61

RMSD from the overall lowest-energy structure 20.0 +/- 0.2

Van der Waals energy -61.6 +/- 5.7

Electrostatic energy -203.5 +/- 66.0


Desolvation energy -7.7 +/- 9.2

Restraints violation energy 241.2 +/- 23.1


Buried Surface Area 1767.9 +/- 249.5


Z-Score 0.1

- Nr 1 best structure




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- Nr 2 best structure



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- Nr 3 best structure



Download file
- Nr 4 best structure



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Cluster 6

HADDOCK score -63.1 +/- 9.1

Cluster size5

RMSD from the overall lowest-energy structure4.7 +/- 0.4

Van der Waals energy-54.8 +/- 6.2

Electrostatic energy-148.5 +/- 49.1

Desolvation energy-11.7 +/- 3.7

Restraints violation energy331.4 +/- 59.8

Buried Surface Area1759.5 +/- 80.1

Z-Score2.0

Nr 1 best structure

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Nr 2 best structure

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Nr 3 best structure

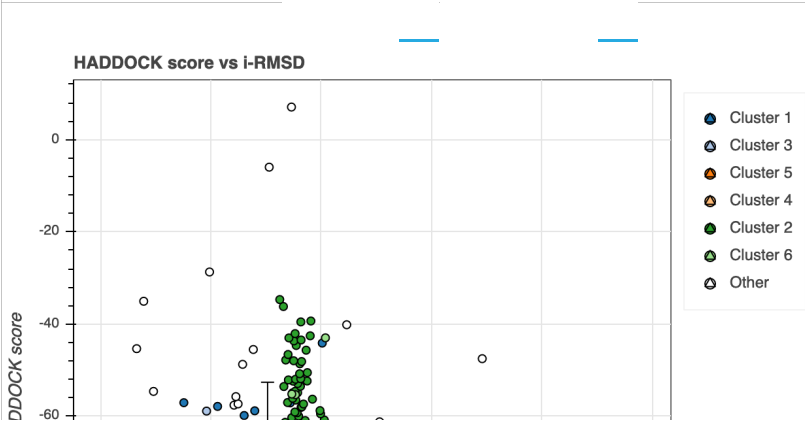
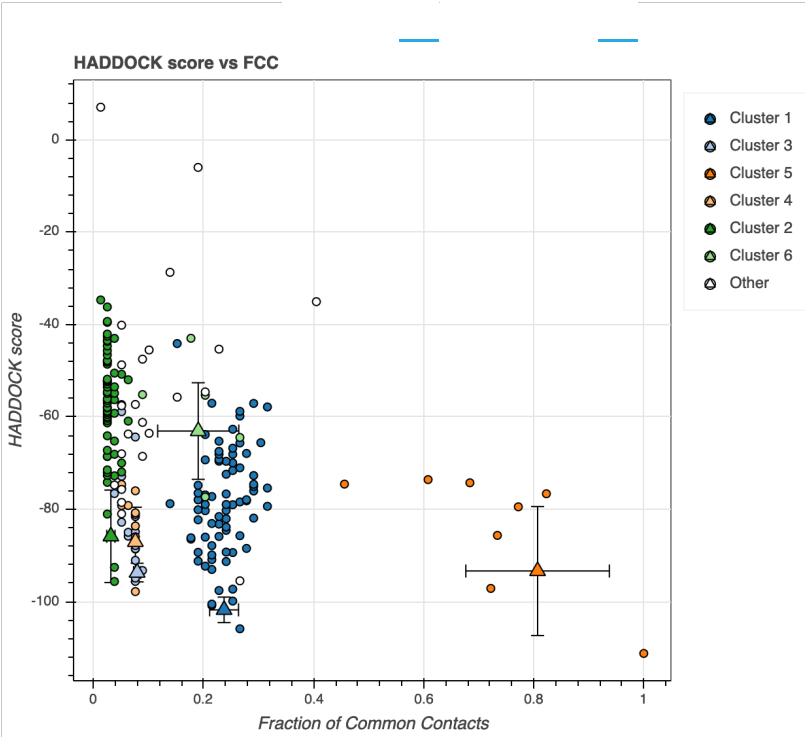
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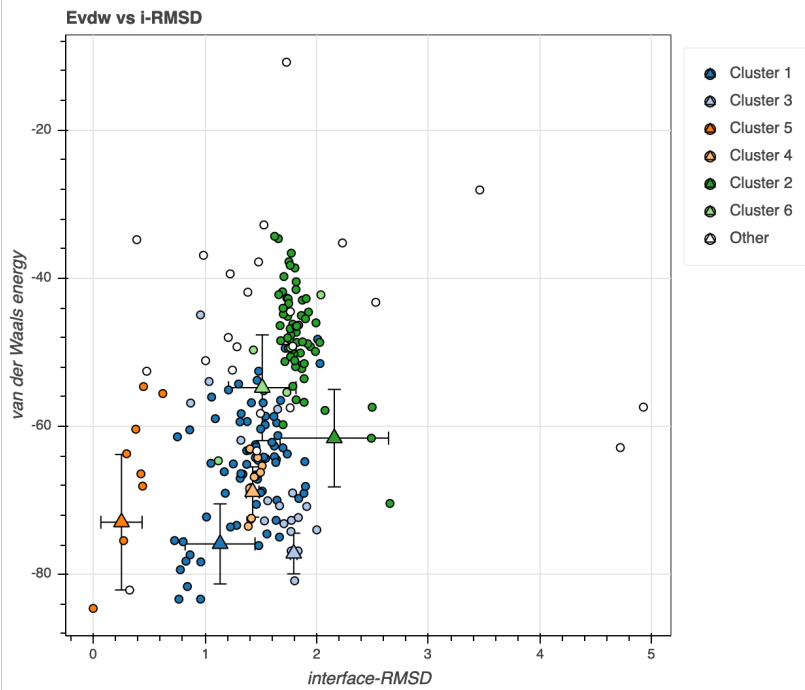
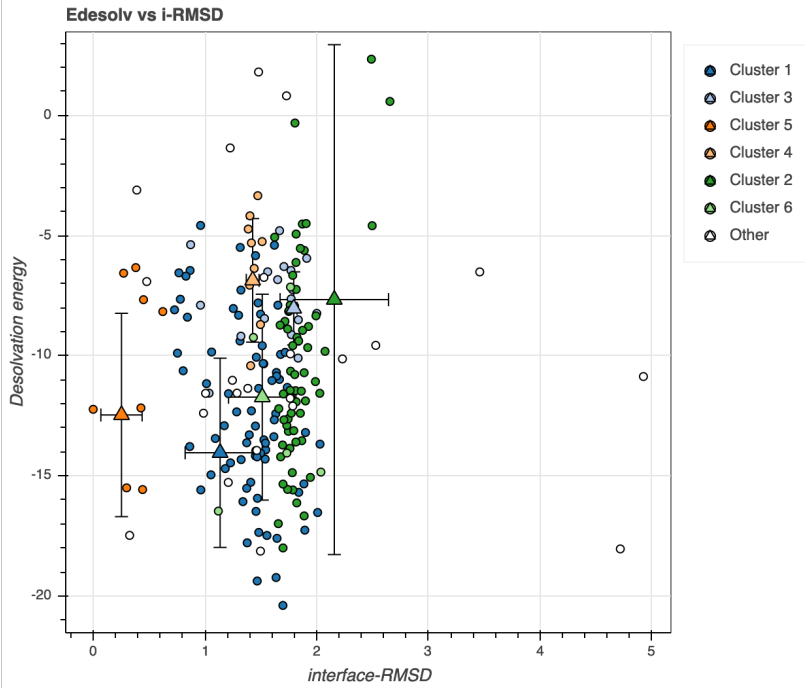
Nr 4 best structure

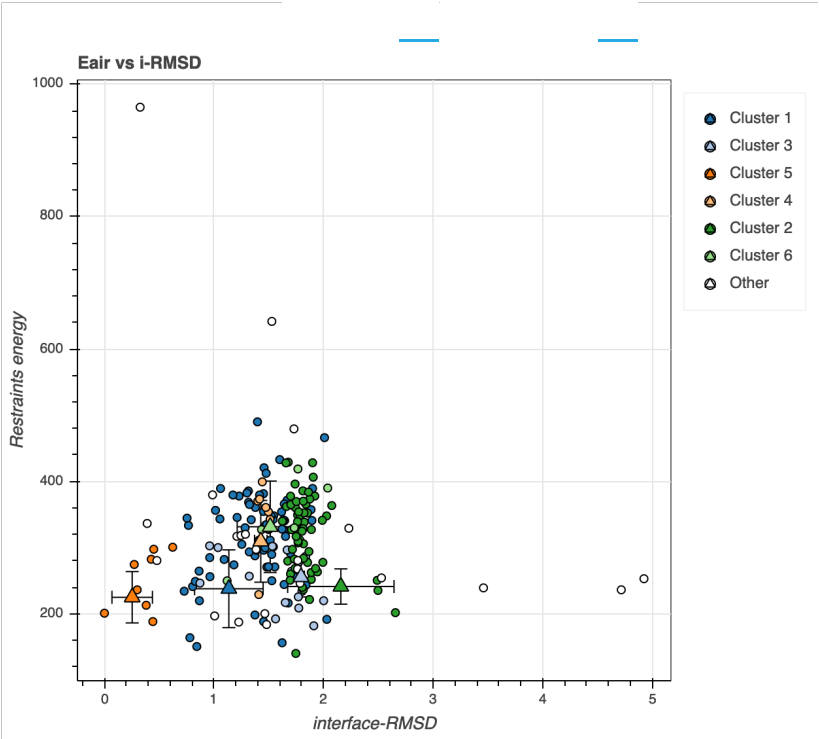
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Model Analysis [\(Download all plots\)](#)

All	None	Cluster 1	Cluster 3	Cluster 5	Cluster 4	Cluster 2	Cluster 6	Other
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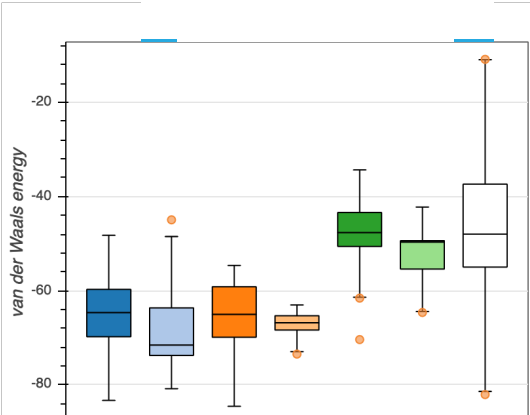


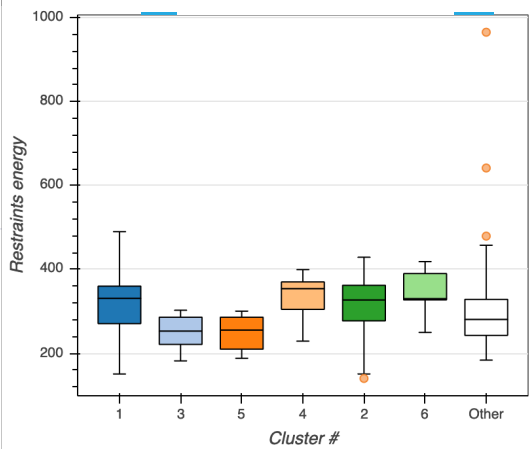
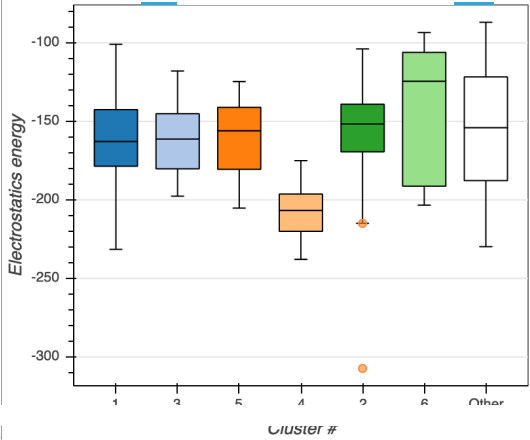




Cluster Analysis

All	None	Cluster 1	Cluster 3	Cluster 5	Cluster 4	Cluster 2	Cluster 6	Other
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