

HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_HLA-csp-15"

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. Kastitis, 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:

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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 **158** structures in **11** cluster(s), which represents **79 %** 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	-78.5 +/- 1.9
Cluster size	67
RMSD from the overall lowest-energy structure	0.4 +/- 0.3
Van der Waals energy	-32.6 +/- 5.8
Electrostatic energy	-143.3 +/- 39.9
Desolvation energy	-17.8 +/- 2.3
Restraints violation energy	5.5 +/- 3.5
Buried Surface Area	1024.8 +/- 22.3
Z-Score	-2.2

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- Nr 2 best structure  [Download file](#)
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Cluster 7

HADDOCK score	-64.4 +/- 1.3
Cluster size	9
RMSD from the overall lowest-energy structure	1.6 +/- 0.0
Van der Waals energy	-25.7 +/- 1.7
Electrostatic energy	-170.9 +/- 13.6
Desolvation energy	-7.3 +/- 1.4
Restraints violation energy	28.1 +/- 25.9
Buried Surface Area	970.2 +/- 111.3
Z-Score	-0.7



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- Nr 3 best structure  [Download file](#)
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Cluster 2


HADDOCK score	-62.0 +/- 2.7
Cluster size	16
RMSD from the overall lowest-energy structure	0.9 +/- 0.1
Van der Waals energy	-32.6 +/- 7.4
Electrostatic energy	-106.0 +/- 22.1
Desolvation energy	-12.0 +/- 5.1
Restraints violation energy	38.2 +/- 14.5
Buried Surface Area	1029.1 +/- 37.1


Z-Score -0.4

- Nr 1 best structure

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Cluster 8

HADDOCK score -60.1 +/- 10.4

Cluster size 6

RMSD from the overall lowest-energy structure 1.3 +/- 0.1

Van der Waals energy -18.9 +/- 6.8

Electrostatic energy -190.9 +/- 40.9



Desolvation energy -5.4 +/- 7.9


Restraints violation energy 24.6 +/- 7.3


Buried Surface Area 920.9 +/- 154.2


Z-Score -0.2

- Nr 1 best structure

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Cluster 5

HADDOCK score -58.6 +/- 3.1

Cluster size 11

RMSD from the overall lowest-energy structure 0.7 +/- 0.1

Van der Waals energy -20.9 +/- 4.6

Electrostatic energy -147.0 +/- 51.2



Desolvation energy -11.6 +/- 3.7


Restraints violation energy 33.1 +/- 15.3


Buried Surface Area 922.7 +/- 33.2


Z-Score -0.1

- Nr 1 best structure

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Cluster 6



HADDOCK score -58.1 +/- 6.0



Cluster size	10
RMSD from the overall lowest-energy structure	1.4 +/- 0.2
Van der Waals energy	-23.5 +/- 2.0
Electrostatic energy	-119.6 +/- 42.6
Desolvation energy	-13.3 +/- 2.1
Restraints violation energy	26.5 +/- 14.4
Buried Surface Area	960.3 +/- 89.0
Z-Score	-0.0


- Nr 1 best structure 

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- Nr 2 best structure 

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Cluster 3

HADDOCK score	-57.1 +/- 1.0
Cluster size	13
RMSD from the overall lowest-energy structure	1.3 +/- 0.1
Van der Waals energy	-20.9 +/- 4.4
Electrostatic energy	-131.0 +/- 30.0
Desolvation energy	-10.9 +/- 2.3
Restraints violation energy	9.2 +/- 7.9
Buried Surface Area	888.2 +/- 45.7
Z-Score	0.1


- Nr 1 best structure 

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Cluster 11

HADDOCK score	-48.6 +/- 5.8
Cluster size	4
RMSD from the overall lowest-energy structure	1.2 +/- 0.0
Van der Waals energy	-13.7 +/- 0.8
Electrostatic energy	-132.2 +/- 30.3
Desolvation energy	-12.2 +/- 2.6
Restraints violation energy	36.7 +/- 28.0
Buried Surface Area	814.0 +/- 26.8
Z-Score	1.0

- Nr 1 best structure 

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- Nr 2 best structure

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Cluster 9

HADDOCK score	-47.2 +/- 5.9
Cluster size	6
RMSD from the overall lowest-energy structure	0.9 +/- 0.1
Van der Waals energy	-19.4 +/- 2.9
Electrostatic energy	-96.1 +/- 13.1
Desolvation energy	-10.9 +/- 2.5
Restraints violation energy	24.0 +/- 13.9
Buried Surface Area	832.3 +/- 64.6
Z-Score	1.1

- Nr 1 best structure

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Cluster 4

HADDOCK score	-44.3 +/- 2.6
Cluster size	11
RMSD from the overall lowest-energy structure	1.2 +/- 0.1
Van der Waals energy	-10.9 +/- 4.5
Electrostatic energy	-147.1 +/- 41.2
Desolvation energy	-9.4 +/- 2.0
Restraints violation energy	54.5 +/- 28.4
Buried Surface Area	840.1 +/- 34.5
Z-Score	1.5

- Nr 1 best structure

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- Nr 2 best structure

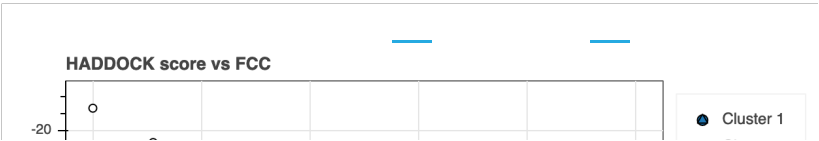
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- Nr 3 best structure

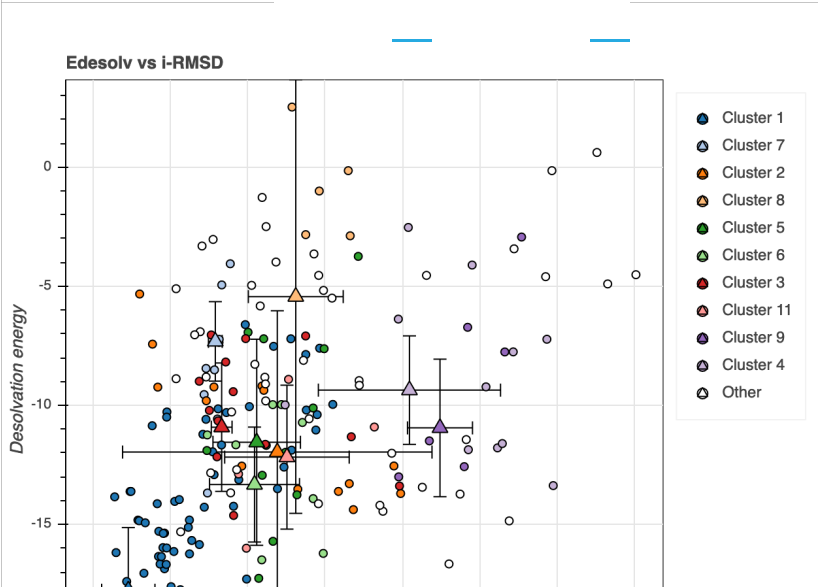
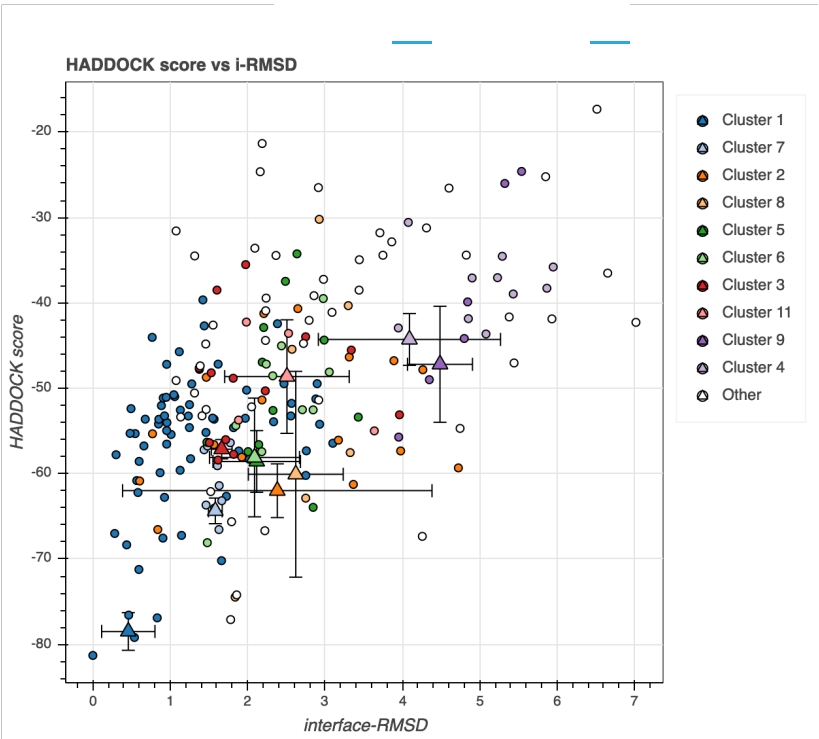
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- Nr 4 best structure

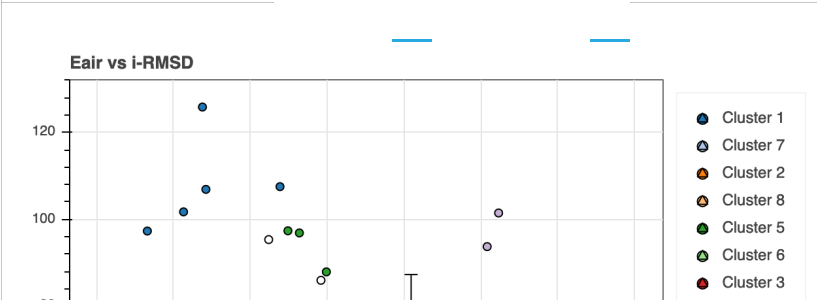
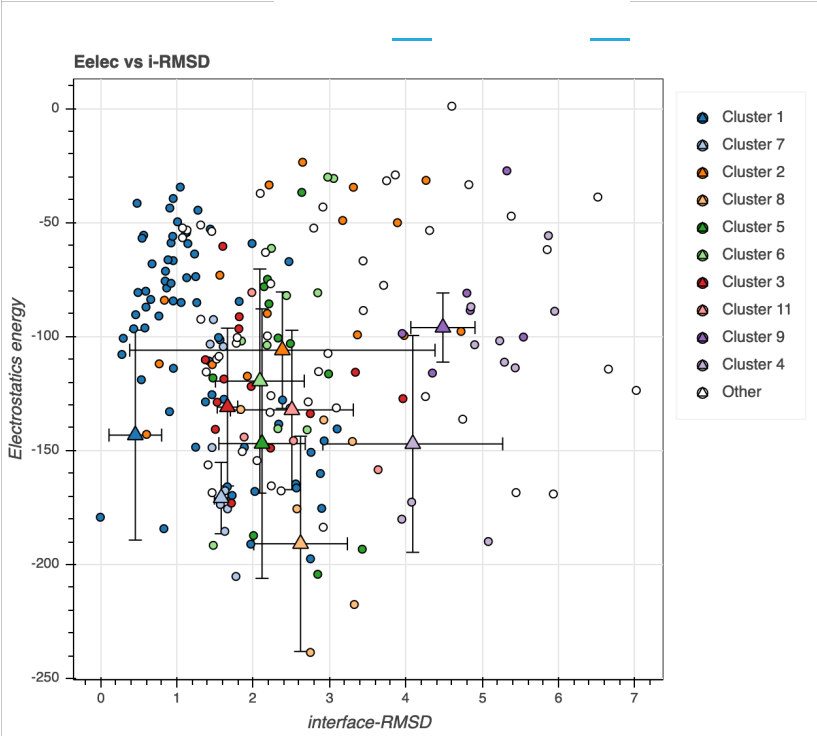
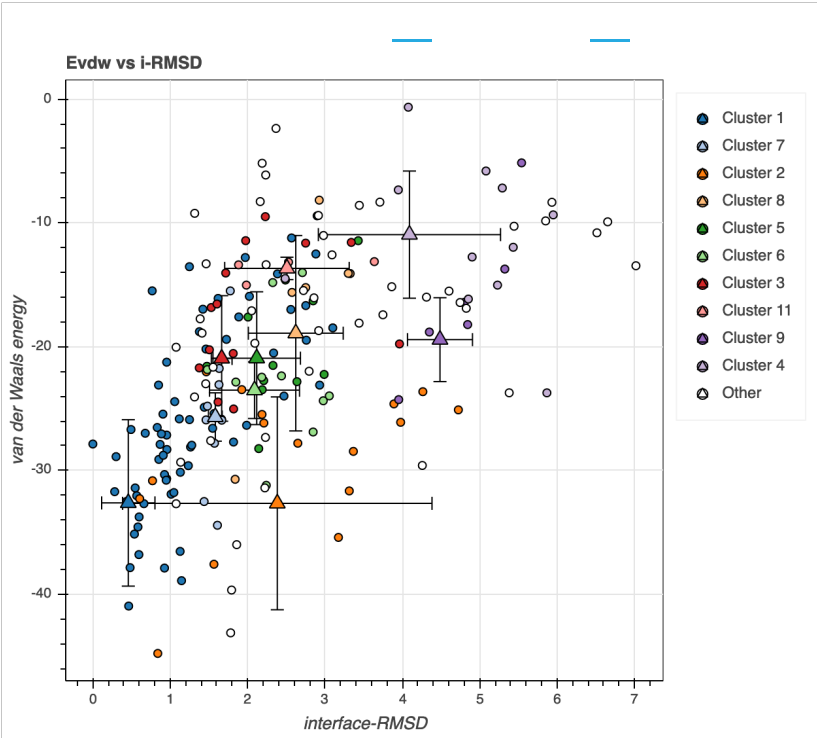
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Model Analysis [\(Download all plots\)](#)

All	None	Cluster 1	Cluster 7	Cluster 2	Cluster 8	Cluster 5	Cluster 6	Cluster 3	Cluster 11	Cluster 9	Cluster 4	C
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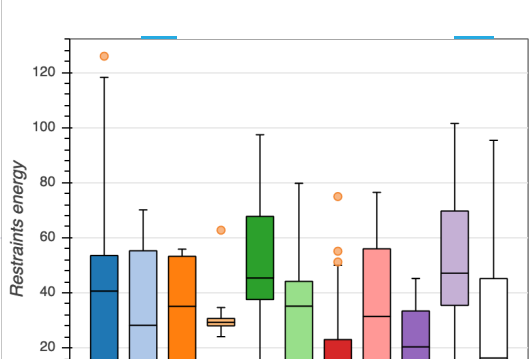
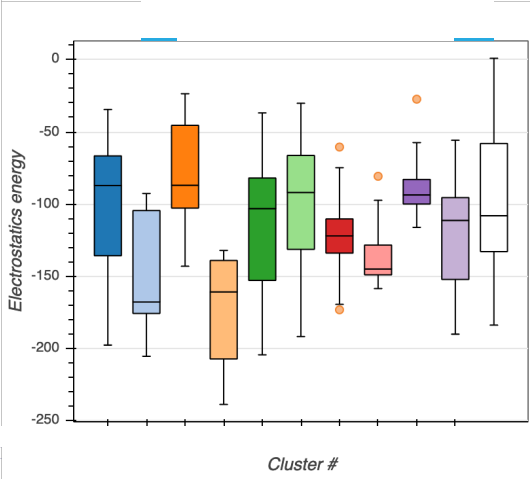
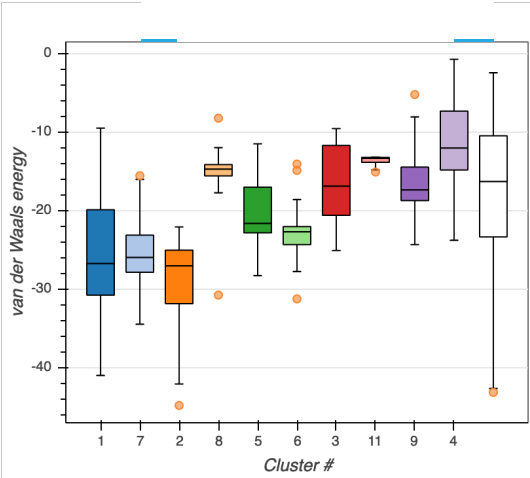






Cluster Analysis

All	None	Cluster 1	Cluster 7	Cluster 2	Cluster 8	Cluster 5	Cluster 6	Cluster 3	Cluster 11	Cluster 9	Cluster 4	O
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