

# HADDOCK 2.4

@Bonvinlab

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## HADDOCK server status for job "cford\_HLA-csp-117"

**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:

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How would you rate your experience with our portal?



Questions / feedback ? [ask.bioexcel.eu](mailto: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 **170** structures in **7** cluster(s), which represents **85 %** 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	-67.6 +/- 2.2
Cluster size	88
RMSD from the overall lowest-energy structure	0.5 +/- 0.3
Van der Waals energy	-34.8 +/- 7.2
Electrostatic energy	-154.9 +/- 43.0
Desolvation energy	-6.5 +/- 1.7
Restraints violation energy	46.1 +/- 30.6
Buried Surface Area	949.0 +/- 28.6
Z-Score	-1.3

Nr 1 best structure		<a href="#">Download file</a>	
Nr 2 best structure		<a href="#">Download file</a>	
Nr 3 best structure		<a href="#">Download file</a>	
Nr 4 best structure		<a href="#">Download file</a>	

**Cluster 3**

HADDOCK score	-57.7 +/- 1.9
Cluster size	19
RMSD from the overall lowest-energy structure	0.8 +/- 0.2
Van der Waals energy	-17.8 +/- 3.3
Electrostatic energy	-188.1 +/- 15.7
Desolvation energy	-4.6 +/- 1.7
Restraints violation energy	22.9 +/- 19.1
Buried Surface Area	887.5 +/- 44.5
Z-Score	-0.6


Nr 1 best structure		<a href="#">Download file</a>	
Nr 2 best structure		<a href="#">Download file</a>	
Nr 3 best structure		<a href="#">Download file</a>	
Nr 4 best structure		<a href="#">Download file</a>	

**Cluster 5**


HADDOCK score	-56.3 +/- 4.0
Cluster size	6
RMSD from the overall lowest-energy structure	0.9 +/- 0.1
Van der Waals energy	-31.0 +/- 5.1
Electrostatic energy	-127.0 +/- 19.4
Desolvation energy	-1.6 +/- 1.9
Restraints violation energy	17.3 +/- 13.4
Buried Surface Area	932.5 +/- 23.9


Z-Score -0.5

- Nr 1 best structure




Download file



- 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 -55.8 +/- 3.7

Cluster size 38

RMSD from the overall lowest-energy structure 1.0 +/- 0.1

Van der Waals energy -24.0 +/- 7.1

Electrostatic energy -149.0 +/- 30.6

Desolvation energy -3.1 +/- 0.8

Restraints violation energy 10.4 +/- 10.1

Buried Surface Area 840.7 +/- 36.7

Z-Score -0.5

- Nr 1 best structure



Download file


- 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 -46.6 +/- 4.5

Cluster size 10

RMSD from the overall lowest-energy structure 1.0 +/- 0.1

Van der Waals energy -18.3 +/- 4.7

Electrostatic energy -137.8 +/- 27.2


Desolvation energy -4.8 +/- 3.7

Restraints violation energy 40.9 +/- 18.3

Buried Surface Area 824.2 +/- 22.7


Z-Score 0.2

- Nr 1 best structure



Download file



- Nr 2 best structure



Download file
- Nr 3 best structure



Download file
- Nr 4 best structure



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Cluster 6

HADDOCK score -41.7 +/- 5.5

Cluster size5

RMSD from the overall lowest-energy structure0.9 +/- 0.1

Van der Waals energy-26.6 +/- 0.8

Electrostatic energy-60.6 +/- 21.4

Desolvation energy-5.7 +/- 1.5

Restraints violation energy27.6 +/- 13.2

Buried Surface Area812.4 +/- 43.8

Z-Score0.6

- 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 7

HADDOCK score-20.5 +/- 7.4

Cluster size4

RMSD from the overall lowest-energy structure1.0 +/- 0.0

Van der Waals energy-10.3 +/- 5.8

Electrostatic energy-53.8 +/- 37.8

Desolvation energy-2.4 +/- 2.3

Restraints violation energy29.9 +/- 14.1

Buried Surface Area591.7 +/- 124.6

Z-Score2.1

- Nr 1 best structure

Download file
- Nr 2 best structure

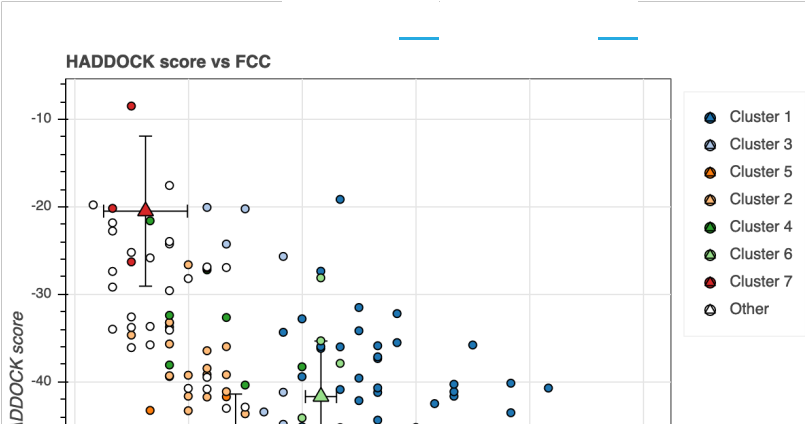
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- Nr 3 best structure

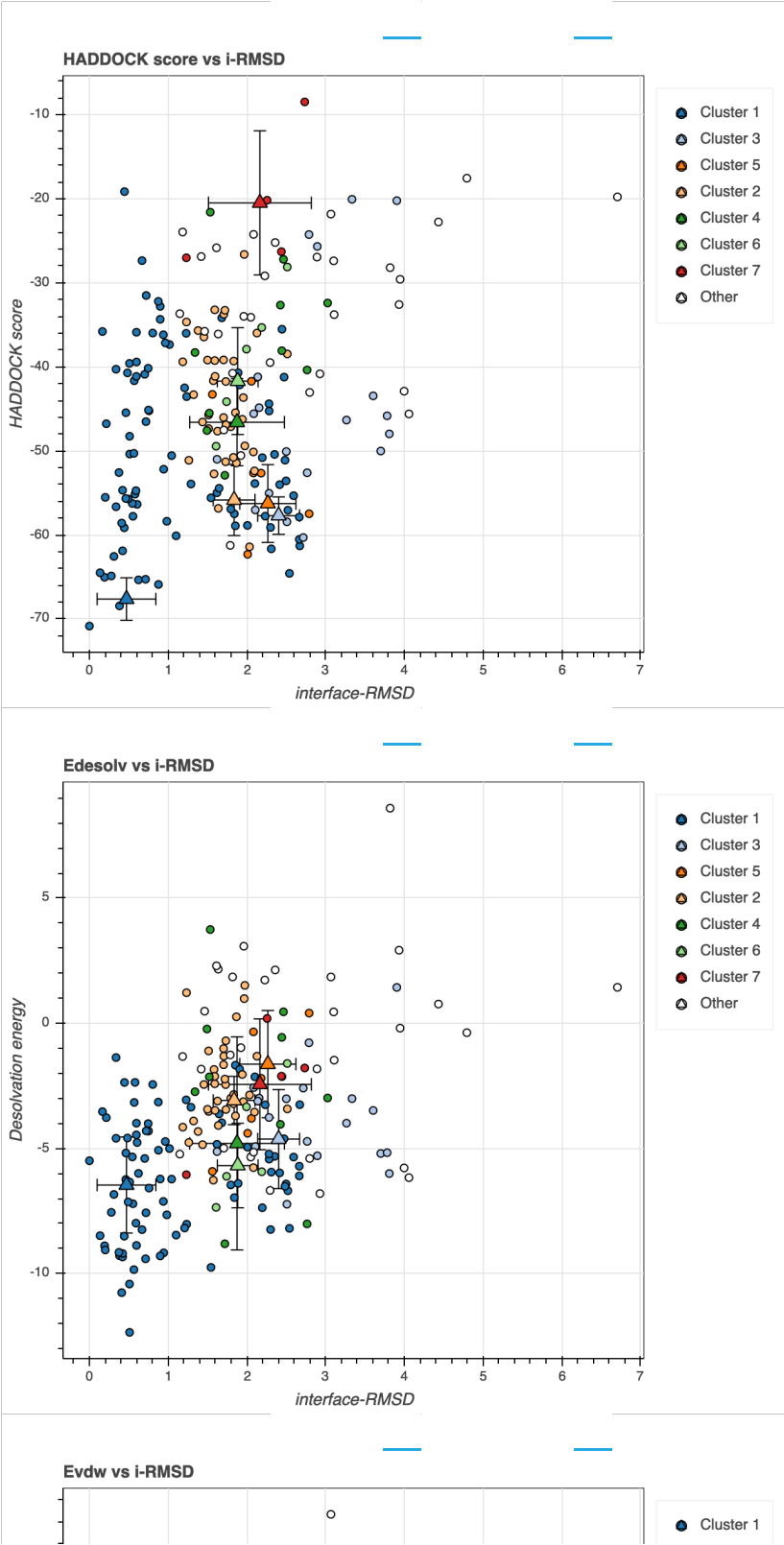
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- Nr 4 best structure

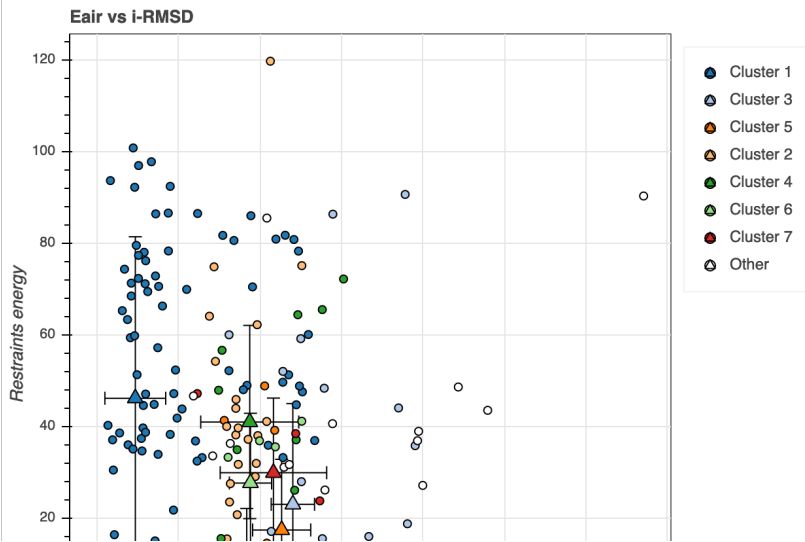
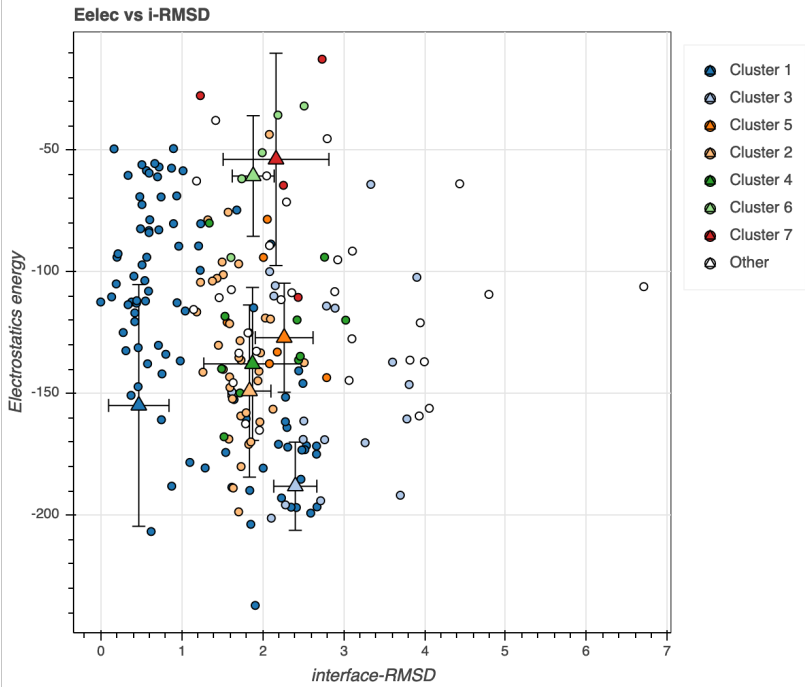
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Model Analysis [\(Download all plots\)](#)

All	None	Cluster 1	Cluster 3	Cluster 5	Cluster 2	Cluster 4	Cluster 6	Cluster 7	Other
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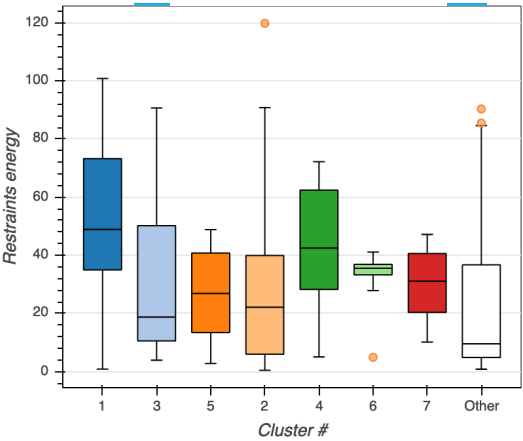
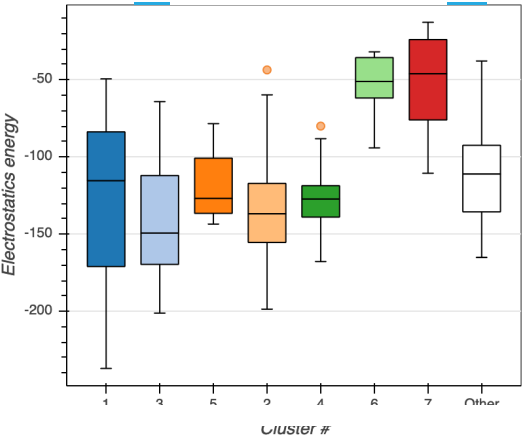
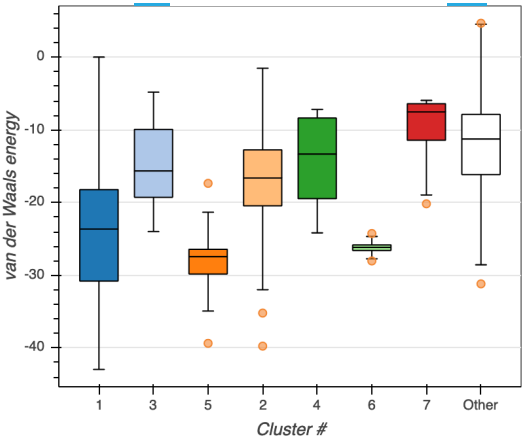






Cluster Analysis

All	None	Cluster 1	Cluster 3	Cluster 5	Cluster 2	Cluster 4	Cluster 6	Cluster 7	Other
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