

# HADDOCK 2.4

@Bonvinlab

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## HADDOCK server status for job "cford\_HLA-csp-94"

**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](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 **178** structures in **11** cluster(s), which represents **89 %** 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	-80.1 +/- 4.9
Cluster size	68
RMSD from the overall lowest-energy structure	0.5 +/- 0.3
Van der Waals energy	-31.1 +/- 6.6
Electrostatic energy	-188.7 +/- 49.2
Desolvation energy	-13.3 +/- 2.7
Restraints violation energy	20.5 +/- 12.0
Buried Surface Area	1323.6 +/- 67.7
Z-Score	-1.4

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- Nr 3 best structure  [Download file](#)
- Nr 4 best structure  [Download file](#)

**Cluster 3**

HADDOCK score	-77.0 +/- 1.5
Cluster size	19
RMSD from the overall lowest-energy structure	0.6 +/- 0.1
Van der Waals energy	-35.3 +/- 1.5
Electrostatic energy	-175.1 +/- 17.0
Desolvation energy	-8.7 +/- 3.3
Restraints violation energy	20.6 +/- 6.5
Buried Surface Area	1478.0 +/- 51.6
Z-Score	-1.0


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**Cluster 4**


HADDOCK score	-76.8 +/- 2.4
Cluster size	14
RMSD from the overall lowest-energy structure	2.6 +/- 0.1
Van der Waals energy	-32.2 +/- 4.8
Electrostatic energy	-164.8 +/- 31.3
Desolvation energy	-13.0 +/- 3.2
Restraints violation energy	13.8 +/- 10.0
Buried Surface Area	1195.1 +/- 53.0


Z-Score -1.0

- Nr 1 best structure




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- Nr 2 best structure



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- Nr 3 best structure



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Cluster 8

HADDOCK score -74.2 +/- 13.7

Cluster size 5

RMSD from the overall lowest-energy structure 2.7 +/- 0.0

Van der Waals energy -29.8 +/- 8.7

Electrostatic energy -192.0 +/- 24.9

Desolvation energy -8.0 +/- 1.2

Restraints violation energy 19.8 +/- 13.9

Buried Surface Area 1398.4 +/- 144.5

Z-Score -0.7

- Nr 1 best structure



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- Nr 3 best structure



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Cluster 2

HADDOCK score -70.0 +/- 1.6

Cluster size 38

RMSD from the overall lowest-energy structure 3.0 +/- 0.0

Van der Waals energy -26.3 +/- 3.2

Electrostatic energy -185.6 +/- 16.9


Desolvation energy -9.7 +/- 1.2

Restraints violation energy 31.6 +/- 29.5

Buried Surface Area 1165.3 +/- 54.0


Z-Score -0.1

- Nr 1 best structure



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- Nr 2 best structure



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- Nr 3 best structure



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Cluster 5

HADDOCK score -69.2 +/- 2.9

Cluster size	10
RMSD from the overall lowest-energy structure	2.8 +/- 0.0
Van der Waals energy	-41.2 +/- 2.9
Electrostatic energy	-84.6 +/- 16.3
Desolvation energy	-14.6 +/- 1.7
Restraints violation energy	36.0 +/- 3.0
Buried Surface Area	1158.6 +/- 82.2
Z-Score	-0.0

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Cluster 6

HADDOCK score	-63.9 +/- 5.8
Cluster size	6
RMSD from the overall lowest-energy structure	2.7 +/- 0.0
Van der Waals energy	-38.4 +/- 5.4
Electrostatic energy	-78.0 +/- 17.7
Desolvation energy	-10.7 +/- 2.5
Restraints violation energy	6.7 +/- 3.2
Buried Surface Area	1347.2 +/- 99.2
Z-Score	0.7

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Cluster 7

HADDOCK score	-63.9 +/- 8.9
Cluster size	6
RMSD from the overall lowest-energy structure	1.0 +/- 0.2
Van der Waals energy	-26.9 +/- 8.2
Electrostatic energy	-139.5 +/- 40.7
Desolvation energy	-10.5 +/- 3.3
Restraints violation energy	13.6 +/- 11.5
Buried Surface Area	1060.8 +/- 81.6
Z-Score	0.7

- Nr 1 best structure

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Cluster 9

HADDOCK score	-58.6 +/- 14.4
Cluster size	4
RMSD from the overall lowest-energy structure	2.9 +/- 0.1
Van der Waals energy	-29.4 +/- 5.0
Electrostatic energy	-93.5 +/- 35.5
Desolvation energy	-11.8 +/- 3.5
Restraints violation energy	12.3 +/- 6.1
Buried Surface Area	1234.7 +/- 215.0
Z-Score	1.4

- Nr 1 best structure

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Cluster 11

HADDOCK score	-56.8 +/- 4.9
Cluster size	4
RMSD from the overall lowest-energy structure	1.1 +/- 0.3
Van der Waals energy	-31.3 +/- 1.4
Electrostatic energy	-91.2 +/- 34.7
Desolvation energy	-13.2 +/- 3.4
Restraints violation energy	59.6 +/- 17.4
Buried Surface Area	1155.2 +/- 92.1
Z-Score	1.6

- Nr 1 best structure

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- Nr 2 best structure

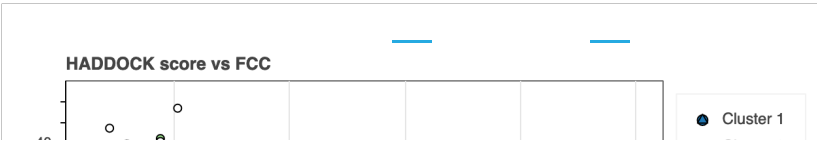
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- Nr 3 best structure

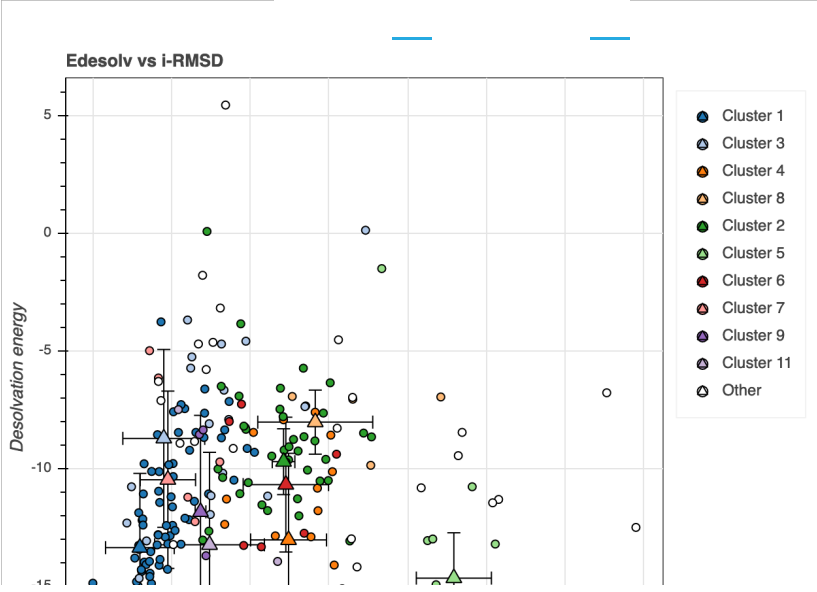
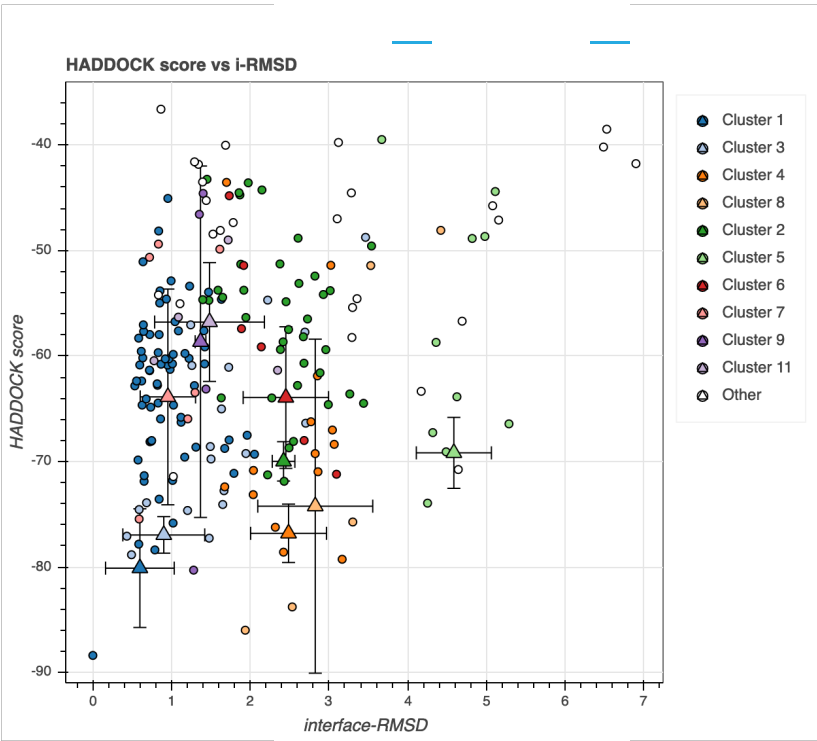
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- Nr 4 best structure

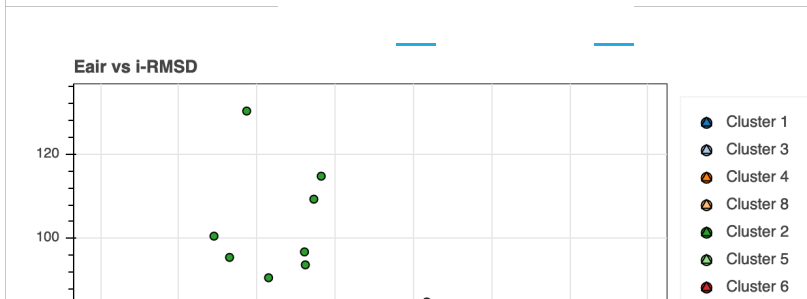
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Model Analysis [\(Download all plots\)](#)

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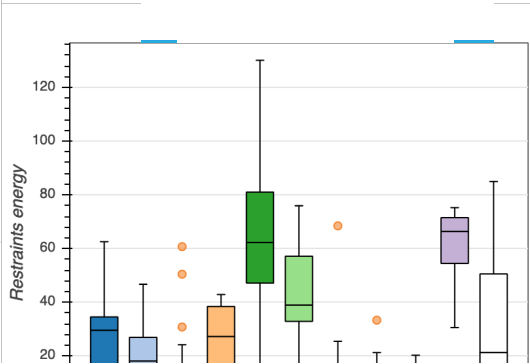
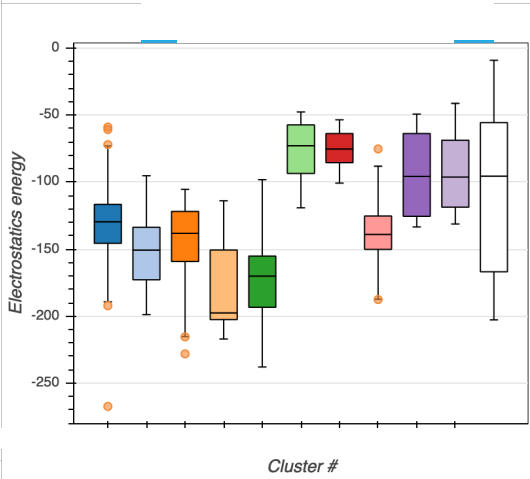
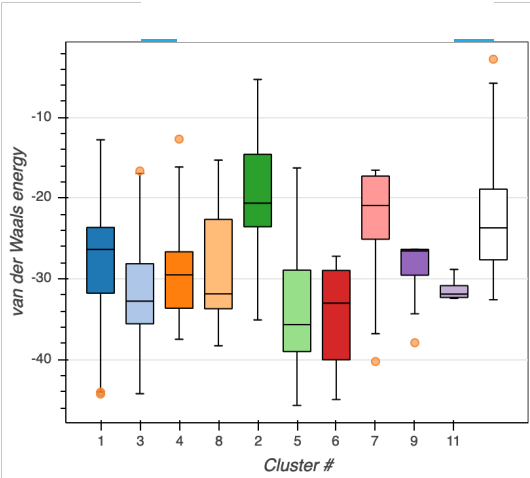






Cluster Analysis

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