

# HADDOCK 2.4

@Bonvinlab

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## HADDOCK server status for job "cford\_TCR-csp-7"

**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 **188** structures in **10** cluster(s), which represents **94 %** 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	-87.5 +/- 2.0
Cluster size	87
RMSD from the overall lowest-energy structure	0.6 +/- 0.4
Van der Waals energy	-74.4 +/- 3.4
Electrostatic energy	-135.9 +/- 22.1
Desolvation energy	-7.0 +/- 3.1
Restraints violation energy	210.5 +/- 35.2
Buried Surface Area	1827.2 +/- 118.9
Z-Score	-1.8

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

HADDOCK score	-83.1 +/- 3.2
Cluster size	35
RMSD from the overall lowest-energy structure	20.0 +/- 0.0
Van der Waals energy	-74.6 +/- 4.2
Electrostatic energy	-113.9 +/- 9.8
Desolvation energy	-8.1 +/- 3.6
Restraints violation energy	223.5 +/- 22.1
Buried Surface Area	2023.9 +/- 75.0
Z-Score	-1.4



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


**Cluster 6**


HADDOCK score	-73.6 +/- 4.9
Cluster size	10
RMSD from the overall lowest-energy structure	15.1 +/- 0.5
Van der Waals energy	-65.2 +/- 2.3
Electrostatic energy	-112.1 +/- 15.2
Desolvation energy	-13.1 +/- 4.4
Restraints violation energy	270.9 +/- 22.1
Buried Surface Area	1735.9 +/- 47.5


Z-Score -0.6

- Nr 1 best structure

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Cluster 10

HADDOCK score -69.9 +/- 0.8

Cluster size 5

RMSD from the overall lowest-energy structure 6.3 +/- 0.3

Van der Waals energy -57.9 +/- 2.5

Electrostatic energy -132.4 +/- 25.9



Desolvation energy -6.8 +/- 3.6


Restraints violation energy 212.6 +/- 53.7


Buried Surface Area 1854.0 +/- 57.8


Z-Score -0.3

- Nr 1 best structure

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Cluster 5

HADDOCK score -69.4 +/- 7.6

Cluster size 11

RMSD from the overall lowest-energy structure 17.6 +/- 0.9

Van der Waals energy -58.6 +/- 5.6

Electrostatic energy -144.7 +/- 17.7



Desolvation energy -6.7 +/- 1.9


Restraints violation energy 248.7 +/- 22.4


Buried Surface Area 2015.2 +/- 71.8


Z-Score -0.3

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Cluster 8



HADDOCK score -60.9 +/- 6.3



Cluster size	6
RMSD from the overall lowest-energy structure	10.1 +/- 0.1
Van der Waals energy	-64.0 +/- 4.3
Electrostatic energy	-81.0 +/- 11.1
Desolvation energy	-10.1 +/- 2.4
Restraints violation energy	294.2 +/- 27.3
Buried Surface Area	1718.1 +/- 95.2
Z-Score	0.5


- Nr 1 best structure 

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- Nr 2 best structure 

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Cluster 9

HADDOCK score	-58.4 +/- 1.4
Cluster size	6
RMSD from the overall lowest-energy structure	17.3 +/- 0.1
Van der Waals energy	-52.1 +/- 3.0
Electrostatic energy	-131.8 +/- 18.1
Desolvation energy	-4.7 +/- 3.1
Restraints violation energy	247.7 +/- 21.3
Buried Surface Area	1708.0 +/- 71.5
Z-Score	0.7


- Nr 1 best structure 

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- Nr 2 best structure 

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Cluster 4

HADDOCK score	-55.1 +/- 3.7
Cluster size	11
RMSD from the overall lowest-energy structure	14.6 +/- 0.1
Van der Waals energy	-46.5 +/- 3.3
Electrostatic energy	-142.4 +/- 22.8
Desolvation energy	-9.5 +/- 1.0
Restraints violation energy	293.6 +/- 22.0
Buried Surface Area	1625.0 +/- 131.7
Z-Score	0.9

- Nr 1 best structure 

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- Nr 2 best structure

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Cluster 7

HADDOCK score	-54.1 +/- 10.7
Cluster size	6
RMSD from the overall lowest-energy structure	4.6 +/- 0.3
Van der Waals energy	-55.6 +/- 5.5
Electrostatic energy	-111.6 +/- 22.0
Desolvation energy	-11.9 +/- 3.9
Restraints violation energy	357.0 +/- 47.9
Buried Surface Area	1784.5 +/- 70.2
Z-Score	1.0

- Nr 1 best structure

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Cluster 3

HADDOCK score	-51.3 +/- 5.3
Cluster size	11
RMSD from the overall lowest-energy structure	9.7 +/- 0.3
Van der Waals energy	-51.0 +/- 8.6
Electrostatic energy	-107.2 +/- 7.4
Desolvation energy	-13.2 +/- 2.5
Restraints violation energy	343.4 +/- 27.2
Buried Surface Area	1456.9 +/- 104.8
Z-Score	1.3

- Nr 1 best structure

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- Nr 2 best structure

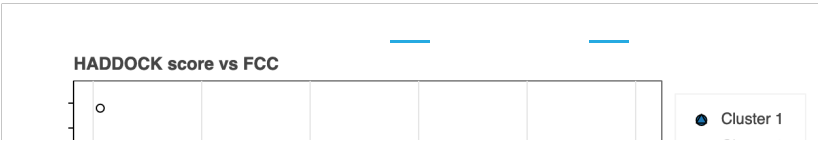
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- Nr 3 best structure

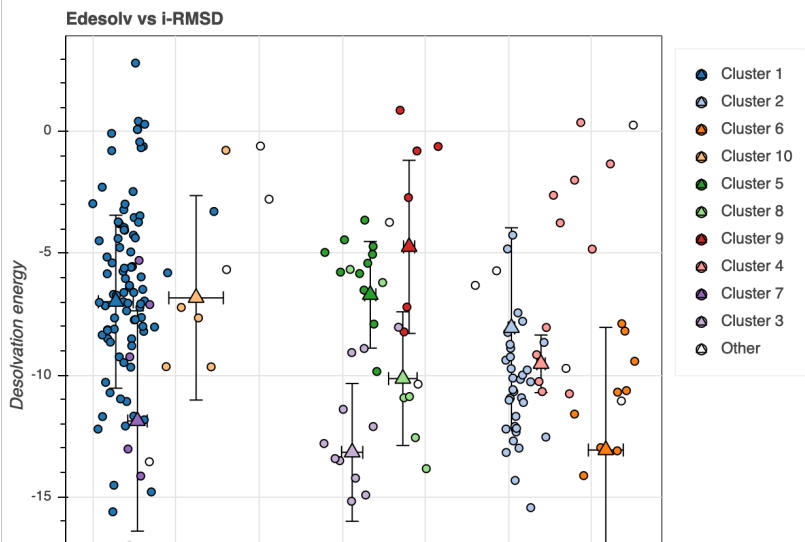
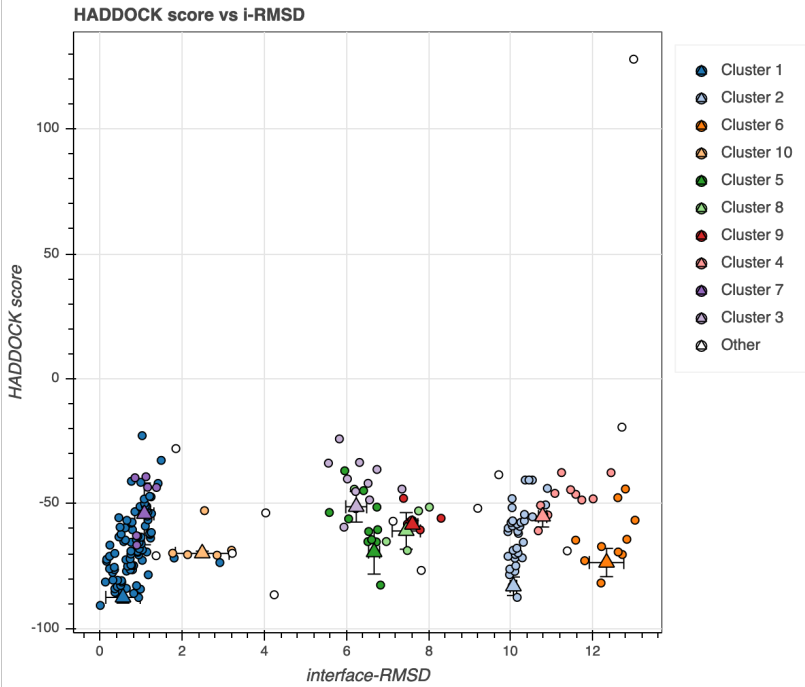
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- Nr 4 best structure

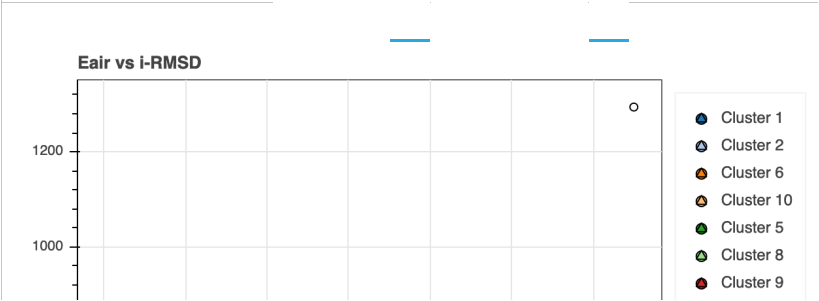
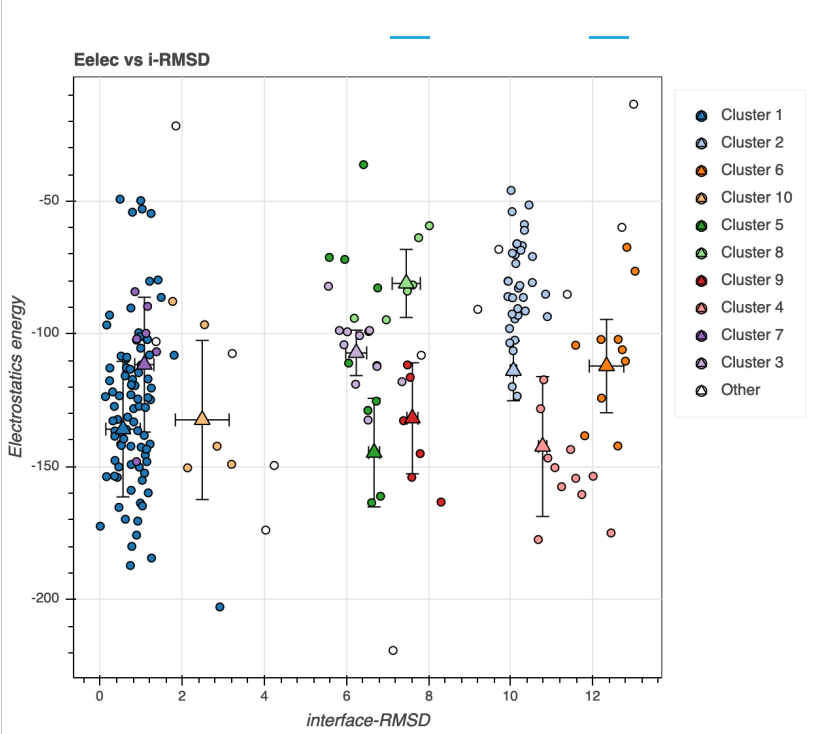
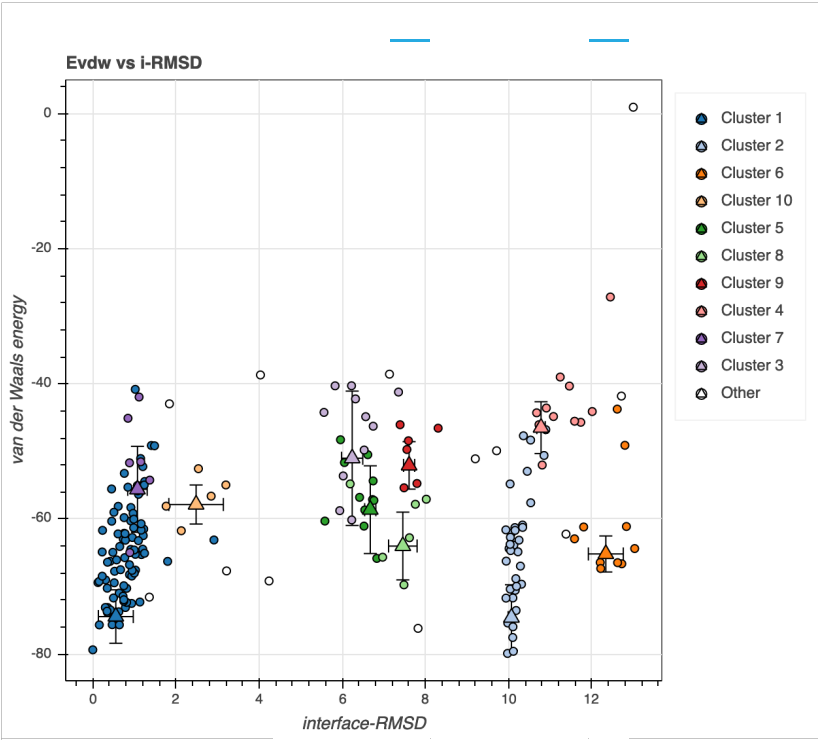
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Model Analysis [\(Download all plots\)](#)

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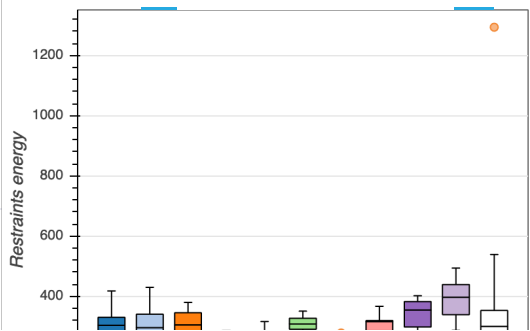
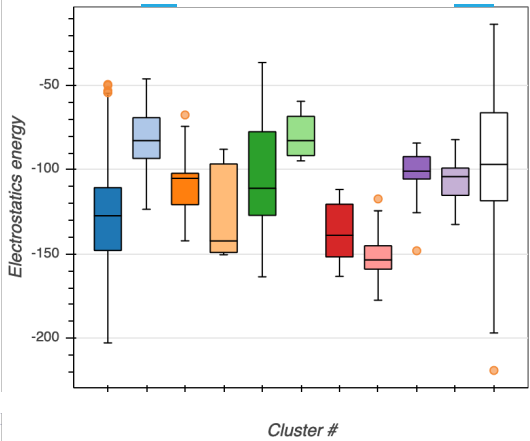
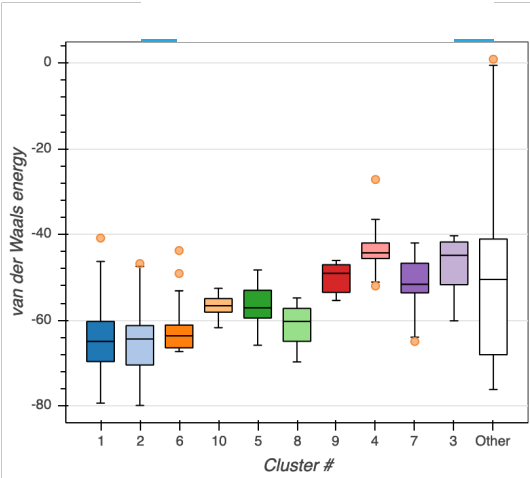






Cluster Analysis

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