HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp_reference"

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. Kastritis, E. Karaca, A.S.J. Melquiond, 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 **183** structures in **9** cluster(s), which represents **91 %** 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 3

HADDOCK score	-96.9 +/- 2.9
Cluster size	38
RMSD from the overall lowest-energy structure	9.6 +/- 1.6
Van der Waals energy	-74.5 +/- 4.3
Electrostatic energy	-190.2 +/- 20.0
Desolvation energy	-1.3 +/- 4.7
Restraints violation energy	169.0 +/- 16.3
Buried Surface Area	2048.1 +/- 46.6
Z-Score	-1.8

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Nr 3 best structure Download file
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Cluster 1

HADDOCK score	-86.2 +/- 11.6
Cluster size	43
RMSD from the overall lowest-energy structure	14.3 +/- 1.0
Van der Waals energy	-66.7 +/- 9.4
Electrostatic energy	-175.0 +/- 15.1
Desolvation energy	-5.3 +/- 2.3
Restraints violation energy	207.8 +/- 31.2
Buried Surface Area	2018.6 +/- 84.5
Z-Score	-1.1

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Cluster 2

HADDOCK score	-80.7 +/- 2.6
Cluster size	38
RMSD from the overall lowest-energy structure	1.8 +/- 0.2
Van der Waals energy	-68.0 +/- 3.7
Electrostatic energy	-171.7 +/- 30.8
Desolvation energy	-8.9 +/- 2.0
Restraints violation energy	305.5 +/- 57.4
Buried Surface Area	1955.8 +/- 39.5

Z-Score	-0.7

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Cluster 4

HADDOCK score	-76.7 +/- 1.5
Cluster size	38
RMSD from the overall lowest-energy structure	17.8 +/- 1.4
Van der Waals energy	-56.3 +/- 6.2
Electrostatic energy	-204.4 +/- 21.8
Desolvation energy	-3.4 +/- 1.8
Restraints violation energy	239.5 +/- 37.6
Buried Surface Area	1742.7 +/- 88.1
Z-Score	-0.4

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Cluster 5

HADDOCK score	-67.2 +/- 7.2
Cluster size	7
RMSD from the overall lowest-energy structure	7.1 +/- 0.2
Van der Waals energy	-52.6 +/- 2.9
Electrostatic energy	-187.2 +/- 21.8
Desolvation energy	-6.2 +/- 2.2
Restraints violation energy	290.0 +/- 48.3
Buried Surface Area	1525.9 +/- 17.4
Z-Score	0.3

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Cluster 8

HADDOCK score	-66.0 +/- 8.8

Cluster size	4
RMSD from the overall lowest-energy structure	16.0 +/- 0.1
Van der Waals energy	-51.0 +/- 5.7
Electrostatic energy	-184.3 +/- 36.7
Desolvation energy	-7.6 +/- 3.4
Restraints violation energy	294.0 +/- 34.6
Buried Surface Area	1656.4 +/- 118.3
Z-Score	0.4

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Cluster 9

HADDOCK score	-60.2 +/- 3.7
Cluster size	4
RMSD from the overall lowest-energy structure	20.7 +/- 0.7
Van der Waals energy	-59.4 +/- 4.2
Electrostatic energy	-113.2 +/- 43.1
Desolvation energy	-6.2 +/- 5.7
Restraints violation energy	280.0 +/- 28.3
Buried Surface Area	1683.2 +/- 10.0
Z-Score	0.8

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Cluster 7

HADDOCK score	-58.9 +/- 10.0
Cluster size	4
RMSD from the overall lowest-energy structure	3.0 +/- 0.1
Van der Waals energy	-57.6 +/- 2.3
Electrostatic energy	-142.7 +/- 38.6
Desolvation energy	-3.0 +/- 2.9
Restraints violation energy	302.6 +/- 14.7
Buried Surface Area	1773.0 +/- 55.0
Z-Score	0.9

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Cluster 6

HADDOCK score	-51.5 +/- 4.7
Cluster size	7
RMSD from the overall lowest-energy structure	5.9 +/- 0.3
Van der Waals energy	-57.6 +/- 2.9
Electrostatic energy	-130.5 +/- 29.5
Desolvation energy	-11.3 +/- 4.1
Restraints violation energy	434.2 +/- 44.5
Buried Surface Area	1502.0 +/- 112.3
Z-Score	1.5

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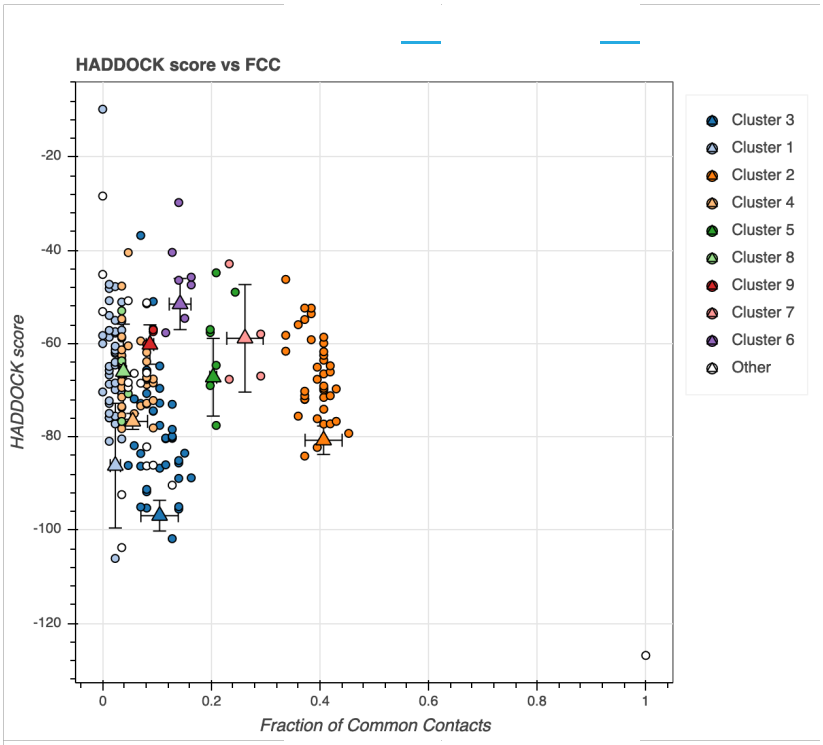
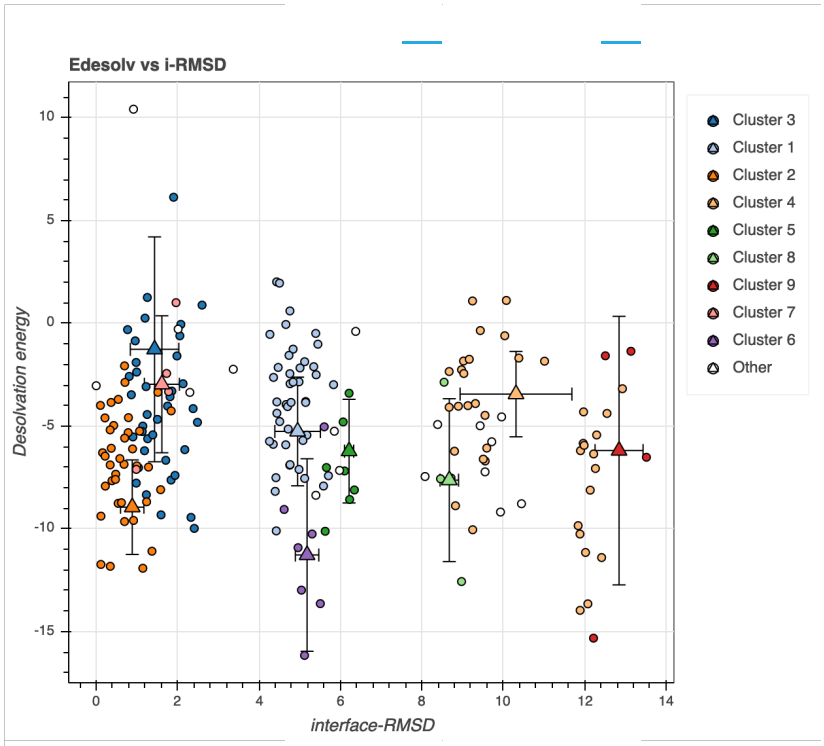
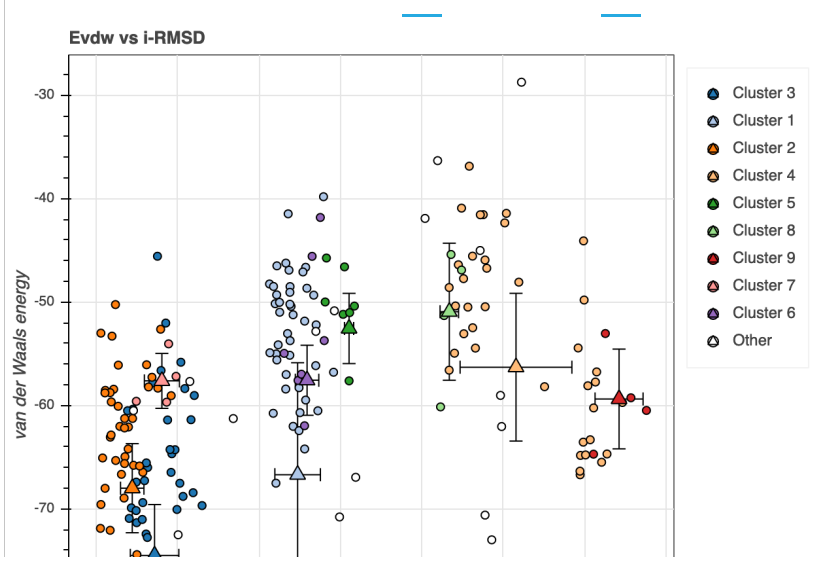
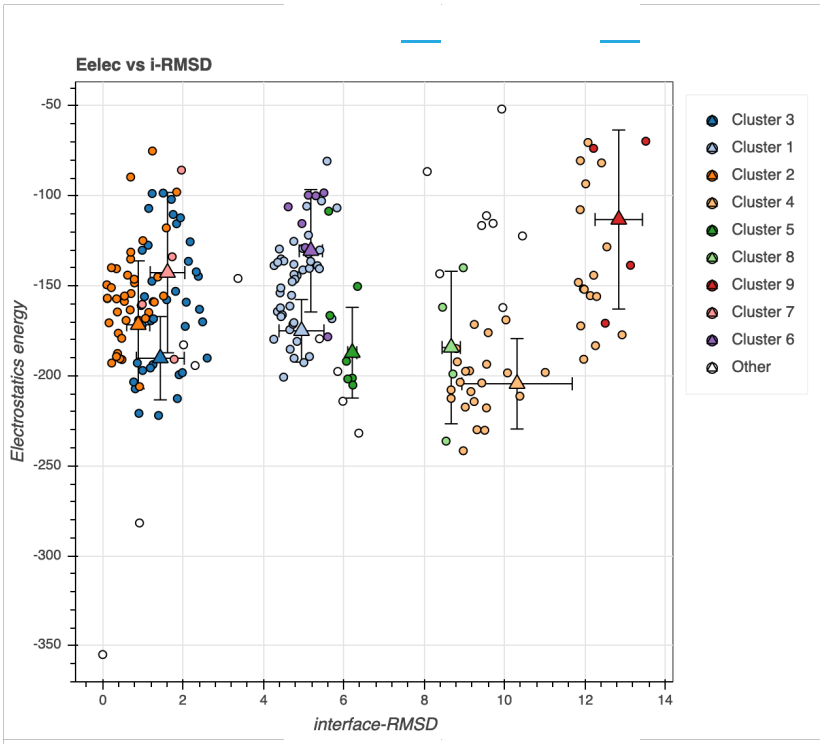
Model Analysis (Download all plots)

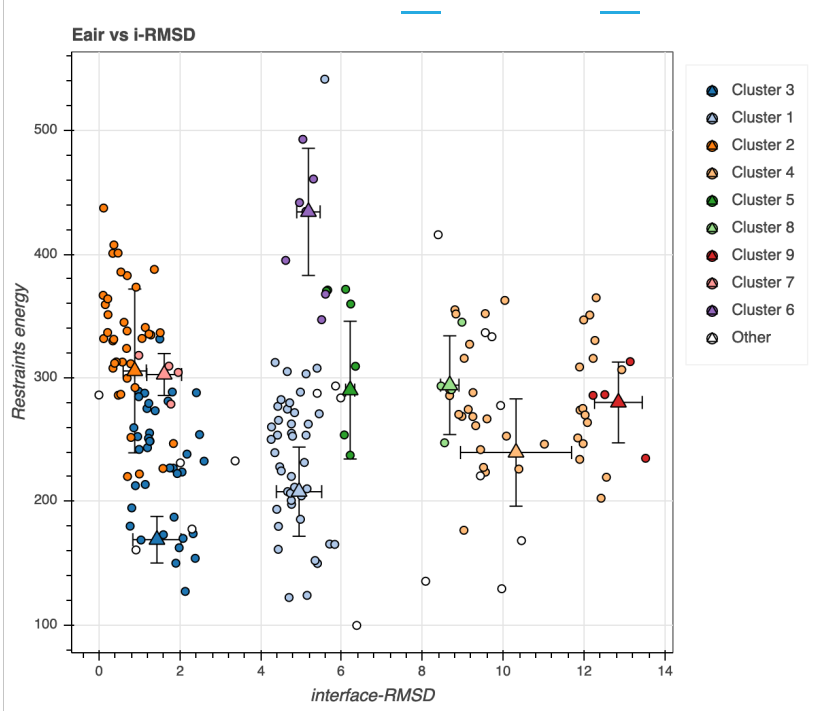
All | None | Cluster 3 | Cluster 1 | Cluster 2 | Cluster 4 | Cluster 5 | Cluster 8 | Cluster 9 | Cluster 7 | Cluster 6 | Ot




Edesolv vs i-RMSD
Desolvation energy
interface-RMSD
Cluster 3
Cluster 1
Cluster 2
Cluster 4
Cluster 5
Cluster 8
Cluster 9
Cluster 7
Cluster 6
Other


Evdw vs i-RMSD
van der Waals energy
Cluster 3
Cluster 1
Cluster 2
Cluster 4
Cluster 5
Cluster 8
Cluster 9
Cluster 7
Cluster 6
Other





Cluster Analysis

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