HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_HLA-csp-35"

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 **173** structures in **9** cluster(s), which represents **86 %** 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 4

HADDOCK score	-76.7 +/- 4.2
Cluster size	20
RMSD from the overall lowest-energy structure	0.5 +/- 0.3
Van der Waals energy	-25.3 +/- 3.7
Electrostatic energy	-246.2 +/- 22.6
Desolvation energy	-4.2 +/- 2.6
Restraints violation energy	20.2 +/- 16.1
Buried Surface Area	1265.3 +/- 67.4
Z-Score	-1.8

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Cluster 2

HADDOCK score	-66.3 +/- 1.5
Cluster size	38
RMSD from the overall lowest-energy structure	2.0 +/- 0.0
Van der Waals energy	-23.2 +/- 1.8
Electrostatic energy	-212.0 +/- 14.5
Desolvation energy	-3.1 +/- 1.4
Restraints violation energy	23.8 +/- 12.8
Buried Surface Area	1145.7 +/- 65.1
Z-Score	-0.7

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Cluster 3

HADDOCK score	-66.1 +/- 2.1
Cluster size	23
RMSD from the overall lowest-energy structure	1.1 +/- 0.1
Van der Waals energy	-26.1 +/- 1.7
Electrostatic energy	-195.6 +/- 10.9
Desolvation energy	-1.6 +/- 0.6
Restraints violation energy	7.7 +/- 1.9
Buried Surface Area	1112.4 +/- 43.2

Z-Score	-0.7

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Cluster 1

HADDOCK score	-65.4 +/- 3.3
Cluster size	62
RMSD from the overall lowest-energy structure	0.8 +/- 0.2
Van der Waals energy	-35.8 +/- 4.2
Electrostatic energy	-150.2 +/- 24.2
Desolvation energy	-3.6 +/- 2.4
Restraints violation energy	40.3 +/- 24.9
Buried Surface Area	1220.7 +/- 72.3
Z-Score	-0.6

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Cluster 9

HADDOCK score	-61.1 +/- 3.4
Cluster size	4
RMSD from the overall lowest-energy structure	2.0 +/- 0.1
Van der Waals energy	-29.2 +/- 7.8
Electrostatic energy	-151.4 +/- 56.4
Desolvation energy	-3.7 +/- 1.6
Restraints violation energy	20.0 +/- 11.6
Buried Surface Area	1059.6 +/- 46.0
Z-Score	-0.1

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Cluster 8

HADDOCK score	-58.3 +/- 6.2

Cluster size	4
RMSD from the overall lowest-energy structure	1.3 +/- 0.2
Van der Waals energy	-32.5 +/- 3.1
Electrostatic energy	-91.9 +/- 69.5
Desolvation energy	-11.0 +/- 4.8
Restraints violation energy	36.2 +/- 17.8
Buried Surface Area	1134.2 +/- 13.1
Z-Score	0.2

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Cluster 5

HADDOCK score	-49.8 +/- 3.5
Cluster size	9
RMSD from the overall lowest-energy structure	1.1 +/- 0.1
Van der Waals energy	-14.5 +/- 6.1
Electrostatic energy	-178.6 +/- 27.7
Desolvation energy	-1.4 +/- 2.7
Restraints violation energy	17.7 +/- 15.5
Buried Surface Area	903.5 +/- 46.7
Z-Score	1.1

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Cluster 6

HADDOCK score	-49.6 +/- 1.5
Cluster size	8
RMSD from the overall lowest-energy structure	0.9 +/- 0.1
Van der Waals energy	-20.7 +/- 8.0
Electrostatic energy	-178.2 +/- 29.9
Desolvation energy	0.8 +/- 1.7
Restraints violation energy	59.2 +/- 16.7
Buried Surface Area	1133.4 +/- 113.2
Z-Score	1.1

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Cluster 7

HADDOCK score	-46.5 +/- 1.4
Cluster size	5
RMSD from the overall lowest-energy structure	2.0 +/- 0.1
Van der Waals energy	-18.1 +/- 7.3
Electrostatic energy	-140.3 +/- 35.0
Desolvation energy	-1.8 +/- 2.6
Restraints violation energy	14.1 +/- 12.9
Buried Surface Area	948.7 +/- 48.5
Z-Score	1.4

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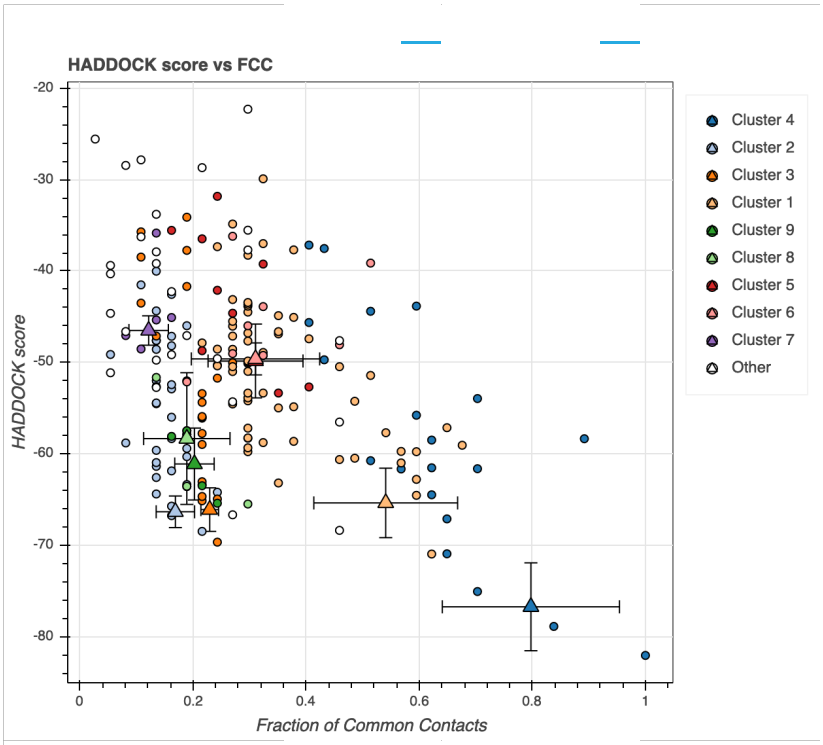
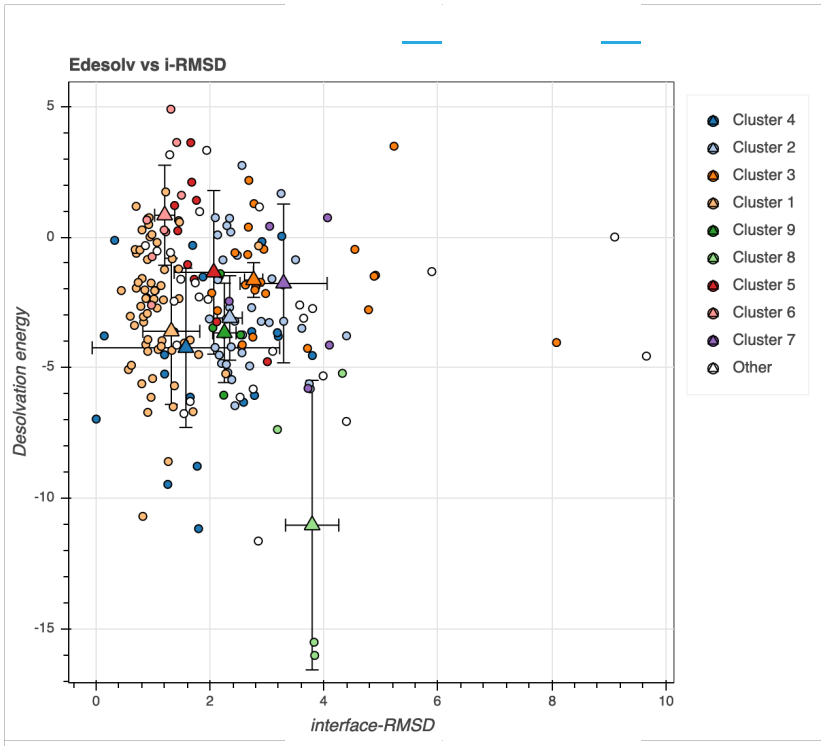
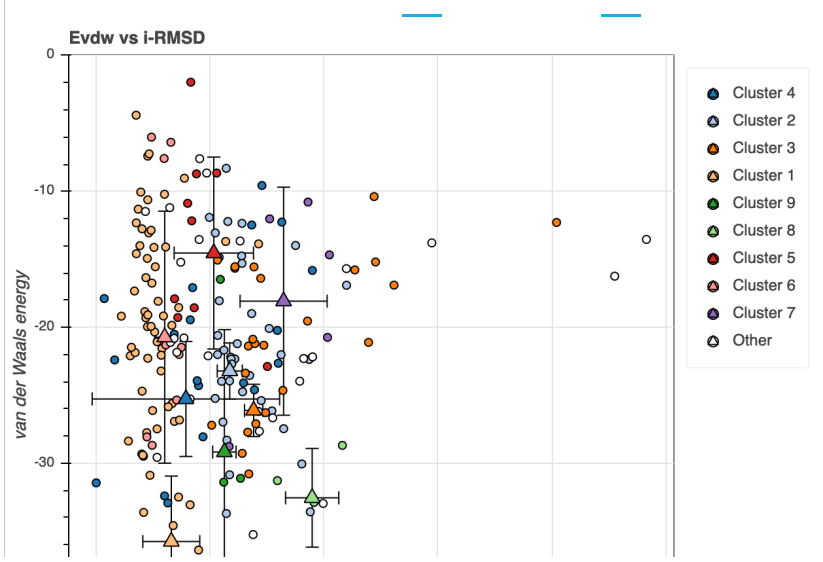
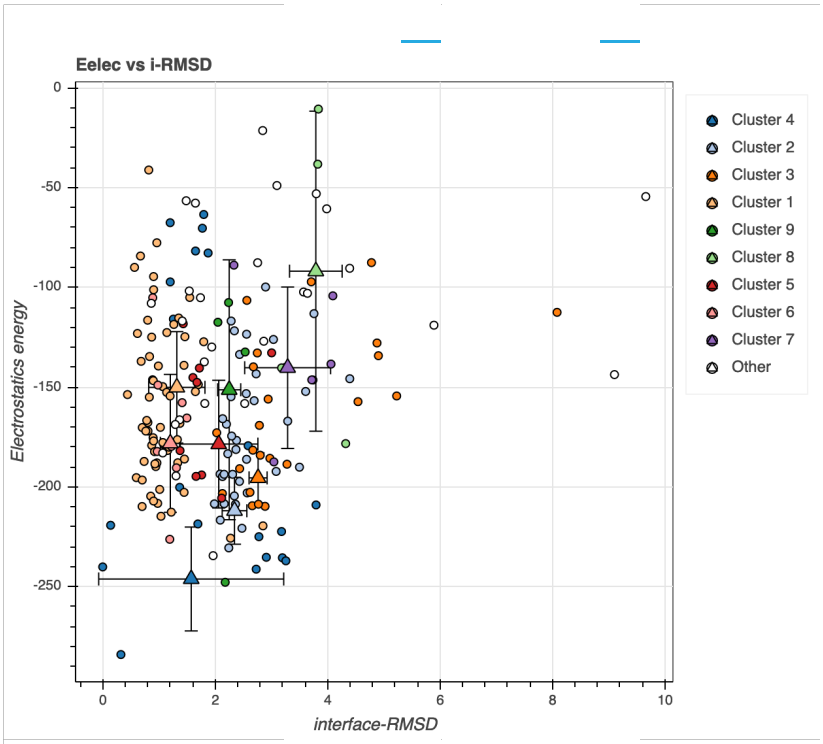
Model Analysis (Download all plots)

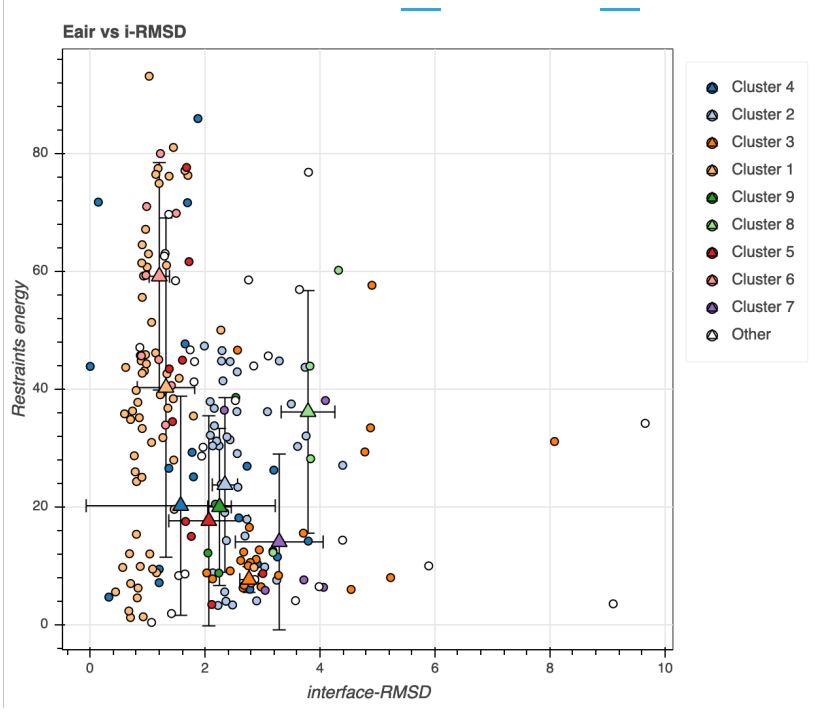
All | None | Cluster 4 | Cluster 2 | Cluster 3 | Cluster 1 | Cluster 9 | Cluster 8 | Cluster 5 | Cluster 6 | Cluster 7 | Ot




Edesolv vs i-RMSD
Desolvation energy
interface-RMSD
5
0
-5
-10
-15
0
2
4
6
8
10
Cluster 4
Cluster 2
Cluster 3
Cluster 1
Cluster 9
Cluster 8
Cluster 5
Cluster 6
Cluster 7
Other


Evdw vs i-RMSD
van der Waals energy
0
-10
-20
-30
Cluster 4
Cluster 2
Cluster 3
Cluster 1
Cluster 9
Cluster 8
Cluster 5
Cluster 6
Cluster 7
Other





Cluster Analysis

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