HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-55"

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:

The FP7 WeNMR (project# 261572), H2020 West-Life (project# 675858), the EOSC-hub (project# 777536) and the EGI-ACE (project# 101017567) European e-Infrastructure projects are acknowledged for the use of their web portals, which make use of the EGI infrastructure with the dedicated support of CESNET-MCC, INFN-PADOVA-STACK, INFN-LNL-2, NCG-INGRID-PT, TW-NCHC, CESGA, IFCA-LCG2, UA-BITP, SURFsara and NIKHEF, and the additional support of the national GRID Initiatives of Belgium, France, Italy, Germany, the Netherlands, Poland, Portugal, Spain, UK, Taiwan and the US Open Science Grid.

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 **186** structures in **5** cluster(s), which represents **93 %** 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	-107.3 +/- 4.7
Cluster size	94
RMSD from the overall lowest-energy structure	1.0 +/- 0.7
Van der Waals energy	-76.9 +/- 6.3
Electrostatic energy	-265.8 +/- 37.5
Desolvation energy	3.0 +/- 5.4
Restraints violation energy	198.5 +/- 49.1
Buried Surface Area	2301.0 +/- 93.0
Z-Score	-1.6

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Cluster 2

HADDOCK score	-83.1 +/- 13.2
Cluster size	58
RMSD from the overall lowest-energy structure	8.2 +/- 0.9
Van der Waals energy	-69.4 +/- 6.3
Electrostatic energy	-161.0 +/- 29.0
Desolvation energy	-4.5 +/- 4.6
Restraints violation energy	230.6 +/- 28.4
Buried Surface Area	2137.3 +/- 108.2
Z-Score	-0.2

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Cluster 3

HADDOCK score	-81.7 +/- 9.0
Cluster size	25
RMSD from the overall lowest-energy structure	10.9 +/- 0.1
Van der Waals energy	-54.0 +/- 6.1
Electrostatic energy	-259.3 +/- 51.5
Desolvation energy	-2.9 +/- 3.9
Restraints violation energy	270.1 +/- 52.5
Buried Surface Area	1820.3 +/- 24.3

Z-Score	-0.1

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Cluster 5

HADDOCK score	-72.4 +/- 5.8
Cluster size	4
RMSD from the overall lowest-energy structure	10.5 +/- 0.4
Van der Waals energy	-59.0 +/- 4.7
Electrostatic energy	-203.6 +/- 27.1
Desolvation energy	-3.7 +/- 3.7
Restraints violation energy	309.8 +/- 33.0
Buried Surface Area	1920.4 +/- 70.3
Z-Score	0.4

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Cluster 4

HADDOCK score	-54.7 +/- 8.5
Cluster size	5
RMSD from the overall lowest-energy structure	22.1 +/- 0.4
Van der Waals energy	-45.7 +/- 0.5
Electrostatic energy	-170.1 +/- 49.5
Desolvation energy	2.4 +/- 4.5
Restraints violation energy	226.4 +/- 45.1
Buried Surface Area	1659.6 +/- 86.5
Z-Score	1.5

Nr 1 best structure   👁   Download file ▾

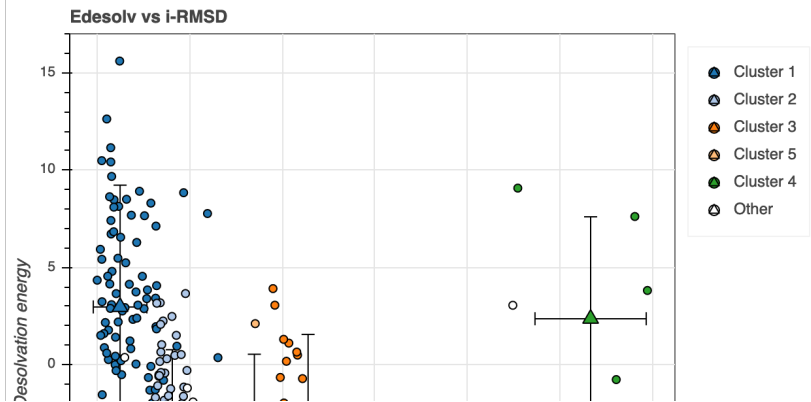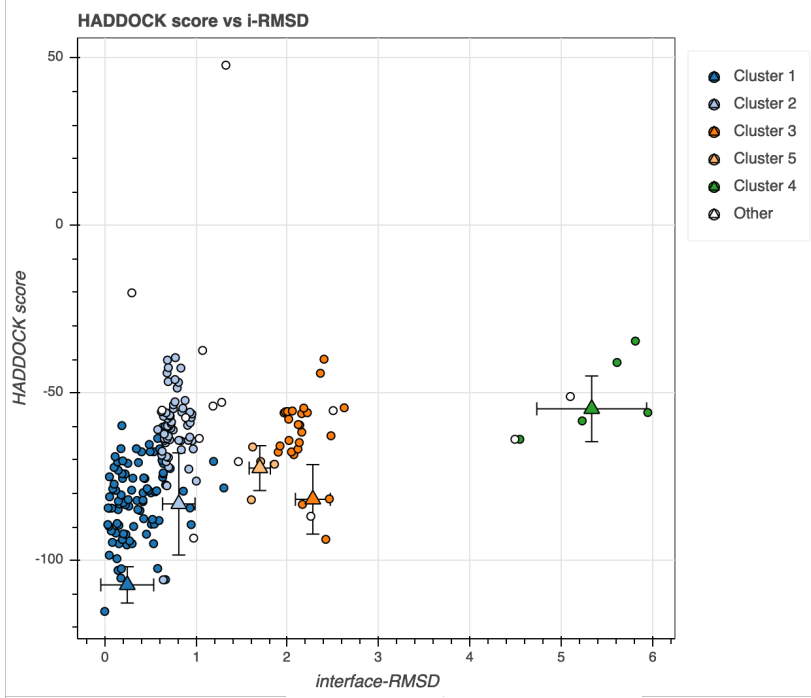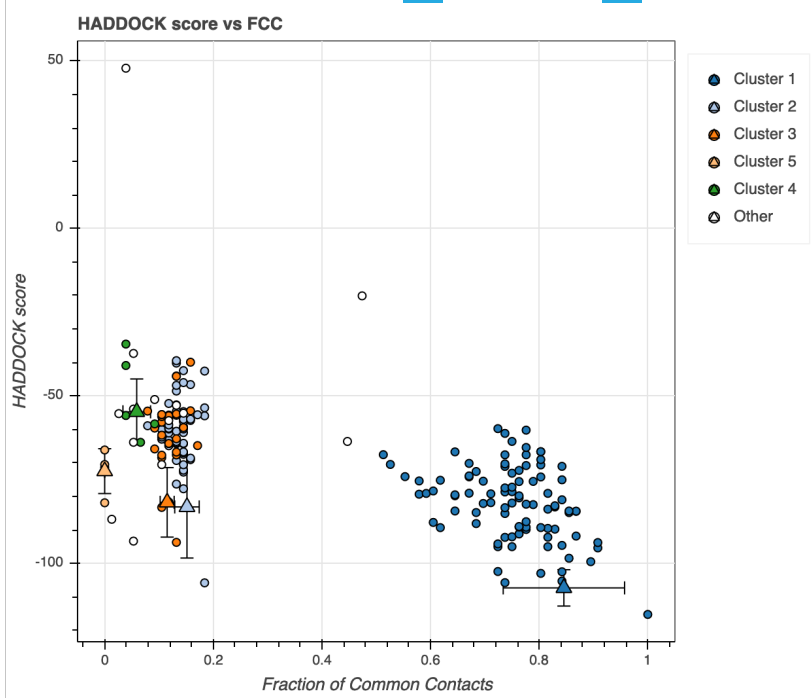Nr 2 best structure   👁   Download file ▾
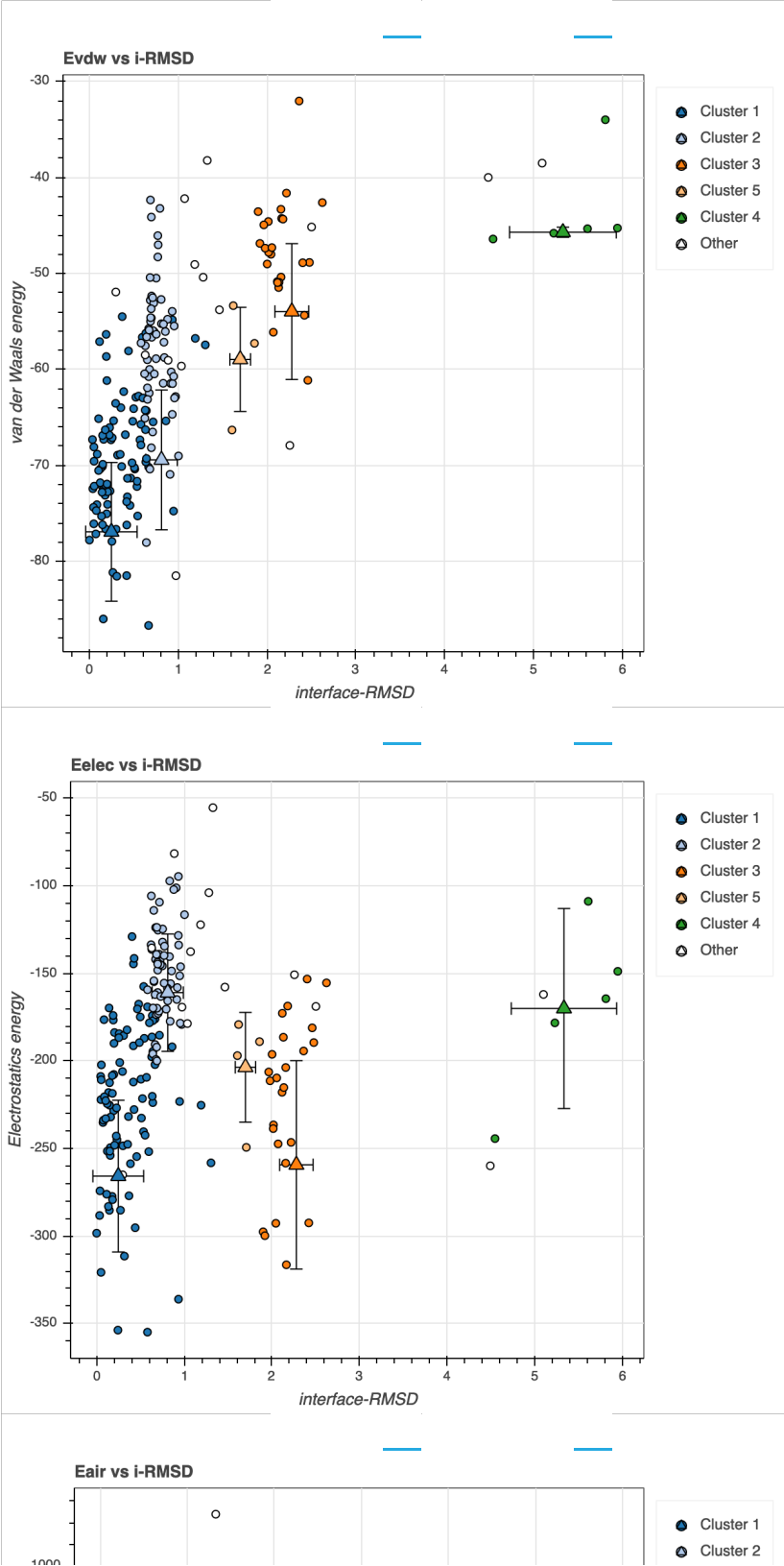
Nr 3 best structure   👁   Download file ▾

Nr 4 best structure   👁   Download file ▾

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

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

HADDOCK score vs FCC

HADDOCK score (y-axis), *Fraction of Common Contacts* (x-axis)

Legend: Cluster 1, Cluster 2, Cluster 3, Cluster 5, Cluster 4, Other

HADDOCK score vs i-RMSD

HADDOCK score (y-axis), *interface-RMSD* (x-axis)

Legend: Cluster 1, Cluster 2, Cluster 3, Cluster 5, Cluster 4, Other

Edesolv vs i-RMSD

Desolvation energy (y-axis)

Legend: Cluster 1, Cluster 2, Cluster 3, Cluster 5, Cluster 4, Other

Evdw vs i-RMSD

Eelec vs i-RMSD

Eair vs i-RMSD
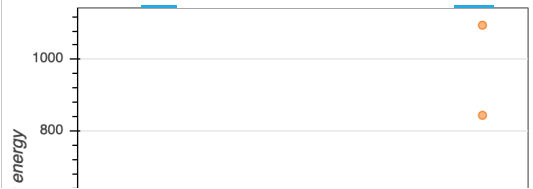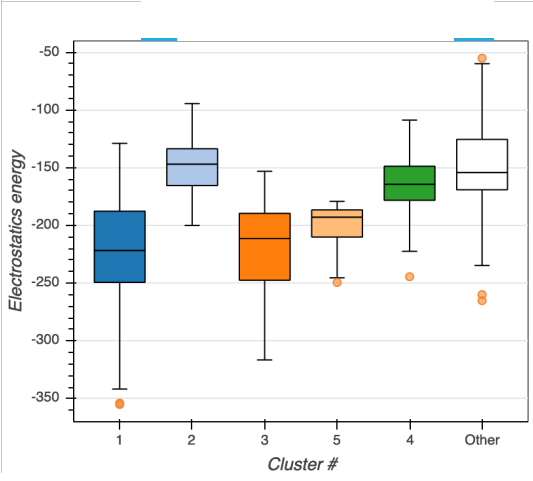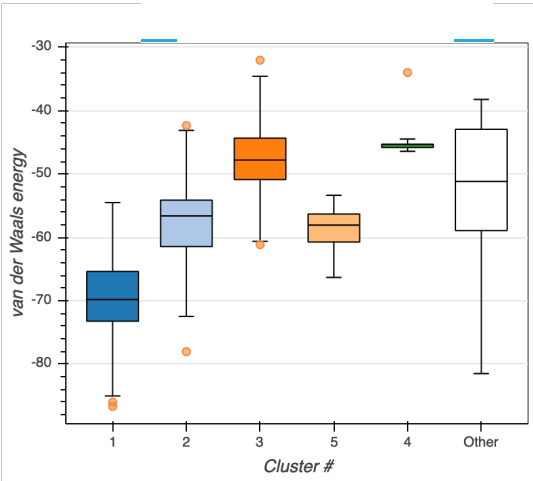
Cluster Analysis

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

...ael Trellet, Jörg Schaarschmidt & Brian Jiménez-García

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