HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-16"

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 **5** 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	-121.7 +/- 2.1
Cluster size	32
RMSD from the overall lowest-energy structure	0.7 +/- 0.6
Van der Waals energy	-79.2 +/- 6.9
Electrostatic energy	-305.5 +/- 22.7
Desolvation energy	-1.6 +/- 3.2
Restraints violation energy	201.9 +/- 62.3
Buried Surface Area	2250.4 +/- 27.9
Z-Score	-1.0

Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 4

HADDOCK score	-116.8 +/- 0.7
Cluster size	29
RMSD from the overall lowest-energy structure	5.5 +/- 0.2
Van der Waals energy	-63.7 +/- 2.3
Electrostatic energy	-363.3 +/- 11.5
Desolvation energy	-3.2 +/- 1.0
Restraints violation energy	227.7 +/- 13.7
Buried Surface Area	1976.5 +/- 21.4
Z-Score	-0.7

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Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 1

HADDOCK score	-116.3 +/- 4.1
Cluster size	73
RMSD from the overall lowest-energy structure	0.8 +/- 0.1
Van der Waals energy	-84.2 +/- 3.9
Electrostatic energy	-264.6 +/- 30.0
Desolvation energy	-3.9 +/- 3.7
Restraints violation energy	246.6 +/- 46.9
Buried Surface Area	2346.2 +/- 61.1

Z-Score	-0.7

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Nr 3 best structure Download file
Nr 4 best structure Download file

Cluster 5

HADDOCK score	-87.8 +/- 6.2
Cluster size	7
RMSD from the overall lowest-energy structure	2.9 +/- 0.1
Van der Waals energy	-72.3 +/- 4.0
Electrostatic energy	-139.4 +/- 24.8
Desolvation energy	-7.5 +/- 2.6
Restraints violation energy	198.5 +/- 68.8
Buried Surface Area	2060.2 +/- 66.3
Z-Score	1.0

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Cluster 2

HADDOCK score	-81.8 +/- 2.0
Cluster size	42
RMSD from the overall lowest-energy structure	7.8 +/- 0.4
Van der Waals energy	-55.3 +/- 3.5
Electrostatic energy	-208.2 +/- 17.4
Desolvation energy	-10.3 +/- 1.9
Restraints violation energy	254.5 +/- 42.0
Buried Surface Area	1611.2 +/- 59.3
Z-Score	1.4

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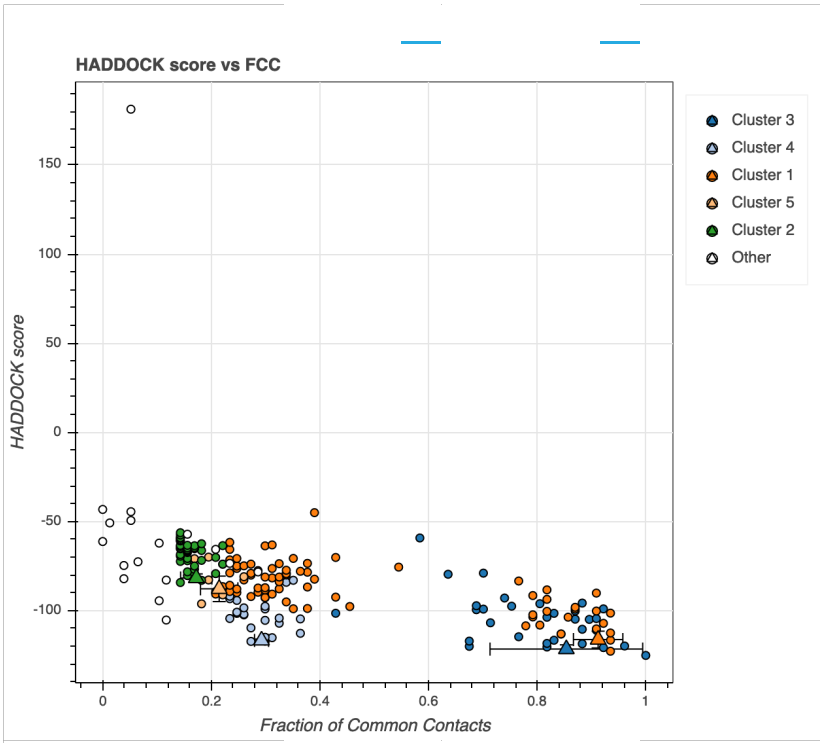
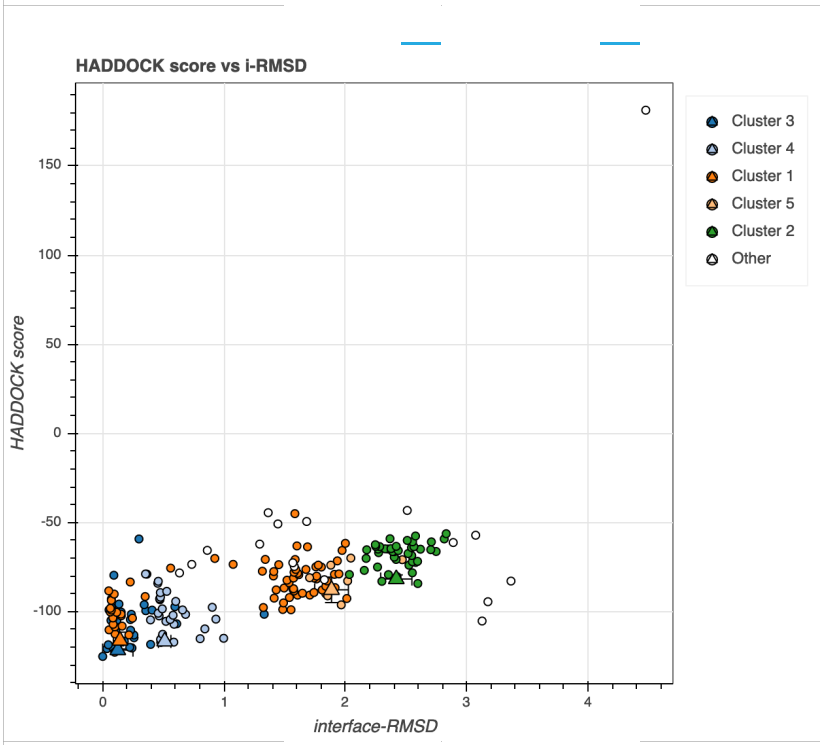
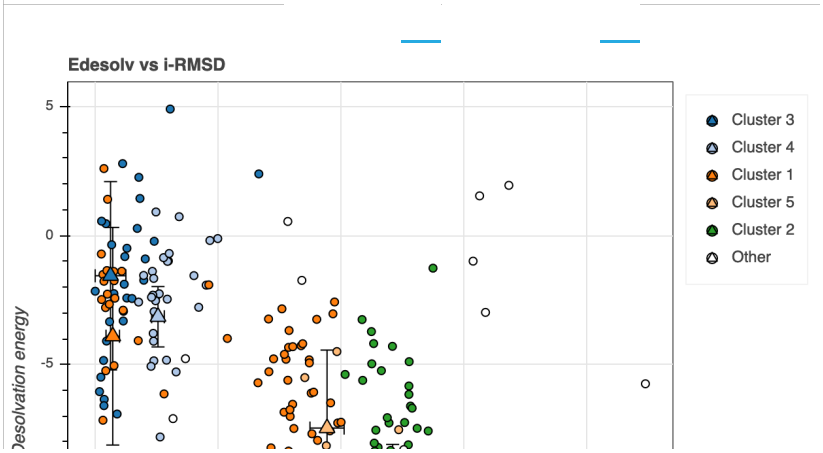
Nr 3 best structure Download file
Nr 4 best structure Download file

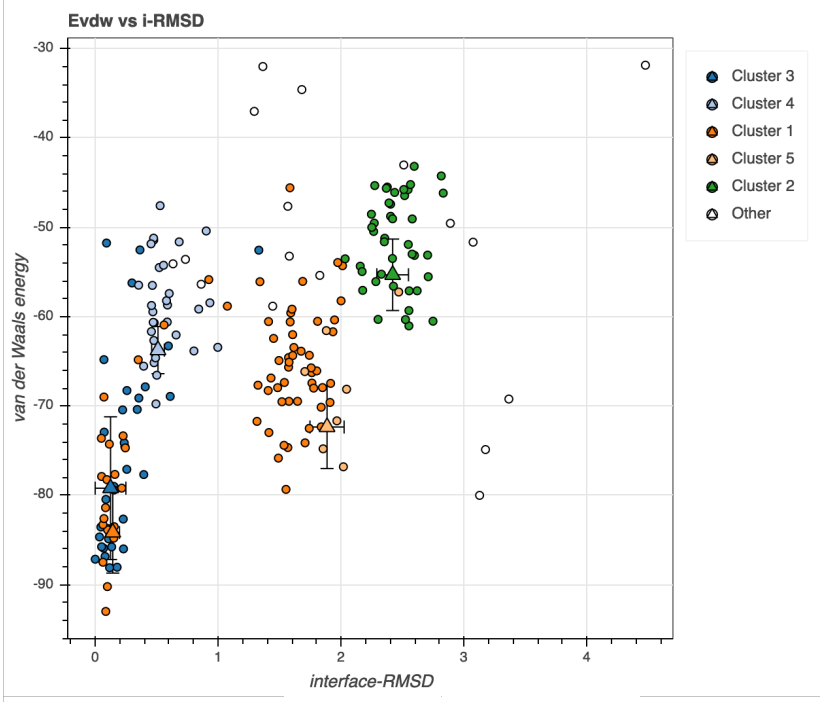
Model Analysis (Download all plots)

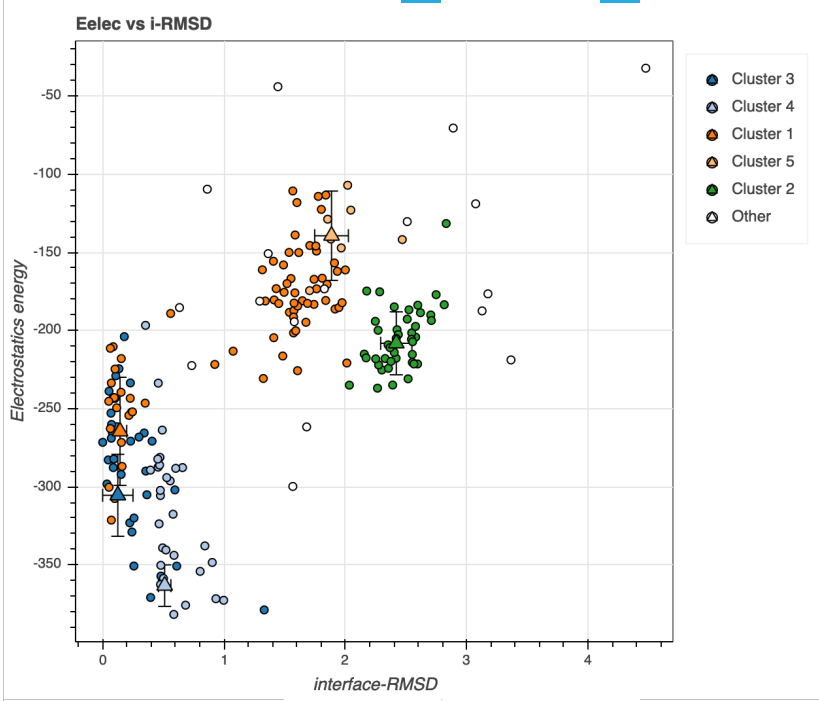
All | None | Cluster 3 | Cluster 4 | Cluster 1 | Cluster 5 | Cluster 2 | Other

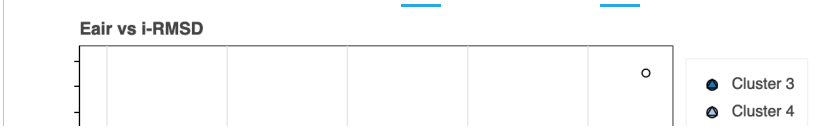

HADDOCK score vs FCC
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Cluster 2
Other
HADDOCK score
150
100
50
0
-50
-100
0
0.2
0.4
0.6
0.8
1
Fraction of Common Contacts


HADDOCK score vs i-RMSD
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Cluster 2
Other
HADDOCK score
150
100
50
0
-50
-100
0
1
2
3
4
interface-RMSD


Edesolv vs i-RMSD
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Cluster 2
Other
5
0
-5

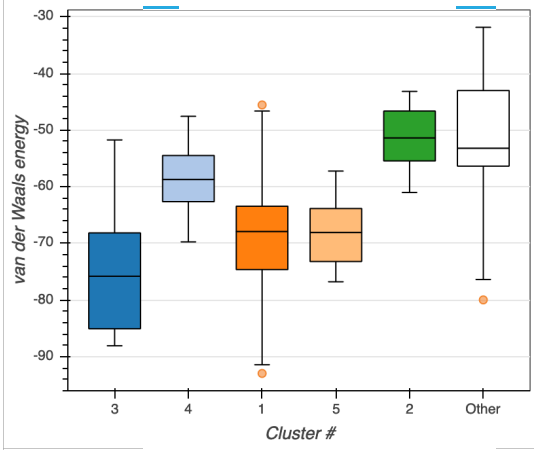

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Cluster 2
Other

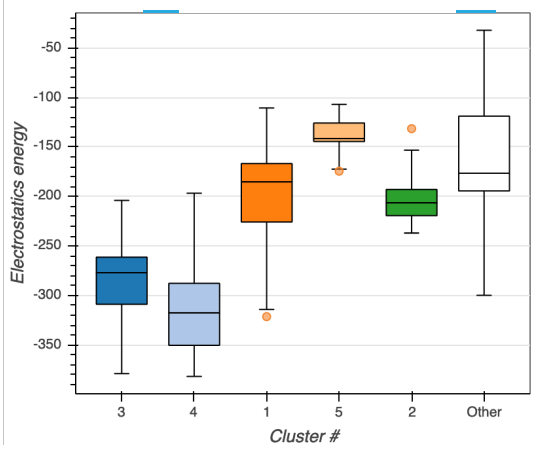

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Cluster 2
Other

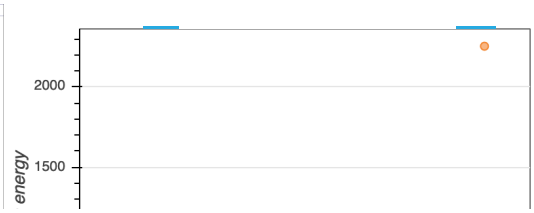

Eair vs i-RMSD
Cluster 3
Cluster 4

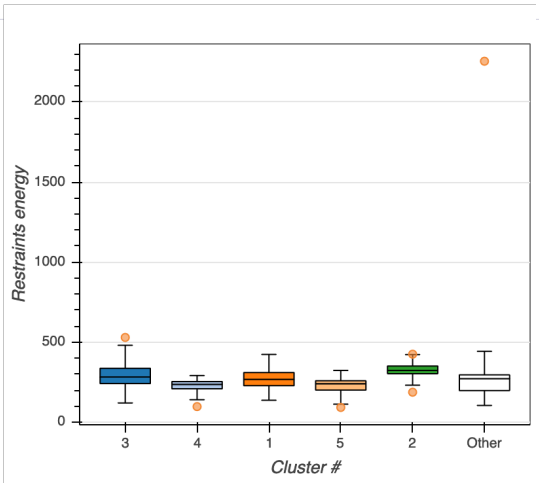
Cluster Analysis

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








Restraints energy
2000
1500
1000
500
0
3
4
1
5
2
Other
Cluster #