HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-94"

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 **191** structures in **5** cluster(s), which represents **95 %** 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 2

HADDOCK score	-94.8 +/- 2.3
Cluster size	68
RMSD from the overall lowest-energy structure	0.5 +/- 0.3
Van der Waals energy	-78.8 +/- 2.8
Electrostatic energy	-152.9 +/- 23.0
Desolvation energy	-6.1 +/- 2.4
Restraints violation energy	207.6 +/- 15.6
Buried Surface Area	1983.3 +/- 81.6
Z-Score	-1.6

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 3

HADDOCK score	-74.2 +/- 1.4
Cluster size	29
RMSD from the overall lowest-energy structure	9.6 +/- 1.0
Van der Waals energy	-71.2 +/- 5.3
Electrostatic energy	-101.6 +/- 23.1
Desolvation energy	-11.2 +/- 4.5
Restraints violation energy	285.7 +/- 33.6
Buried Surface Area	1979.1 +/- 51.2
Z-Score	-0.4

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

Cluster 4

HADDOCK score	-65.1 +/- 3.7
Cluster size	10
RMSD from the overall lowest-energy structure	8.0 +/- 0.4
Van der Waals energy	-62.6 +/- 3.8
Electrostatic energy	-92.2 +/- 9.5
Desolvation energy	-6.9 +/- 4.7
Restraints violation energy	228.1 +/- 59.5
Buried Surface Area	1815.7 +/- 64.7

Z-Score	0.2

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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	-63.9 +/- 2.3
Cluster size	79
RMSD from the overall lowest-energy structure	10.4 +/- 1.2
Van der Waals energy	-65.8 +/- 1.6
Electrostatic energy	-97.6 +/- 12.6
Desolvation energy	-10.9 +/- 3.4
Restraints violation energy	323.4 +/- 50.4
Buried Surface Area	1965.2 +/- 79.1
Z-Score	0.3

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

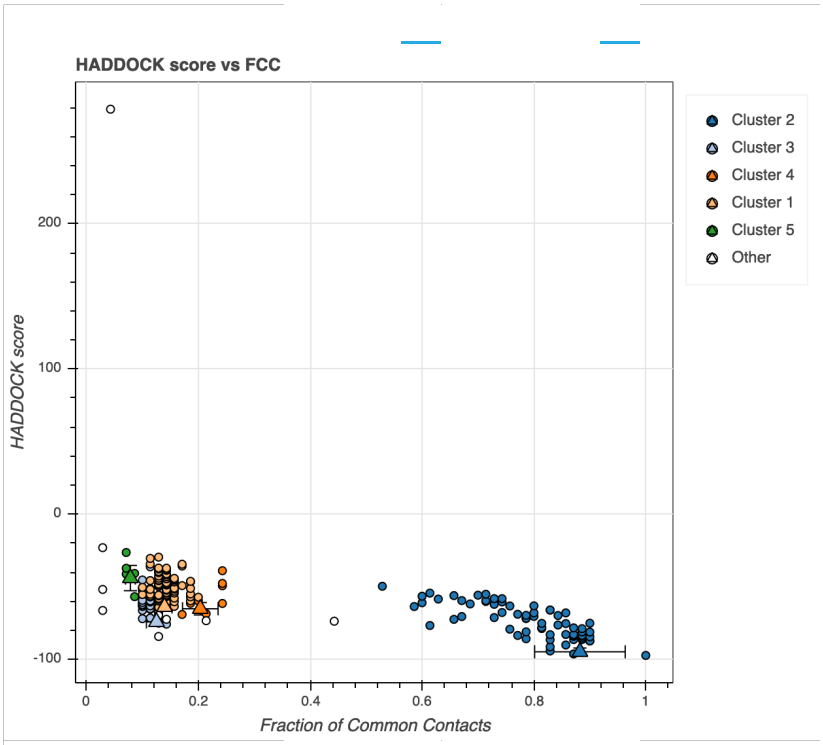
Cluster 5

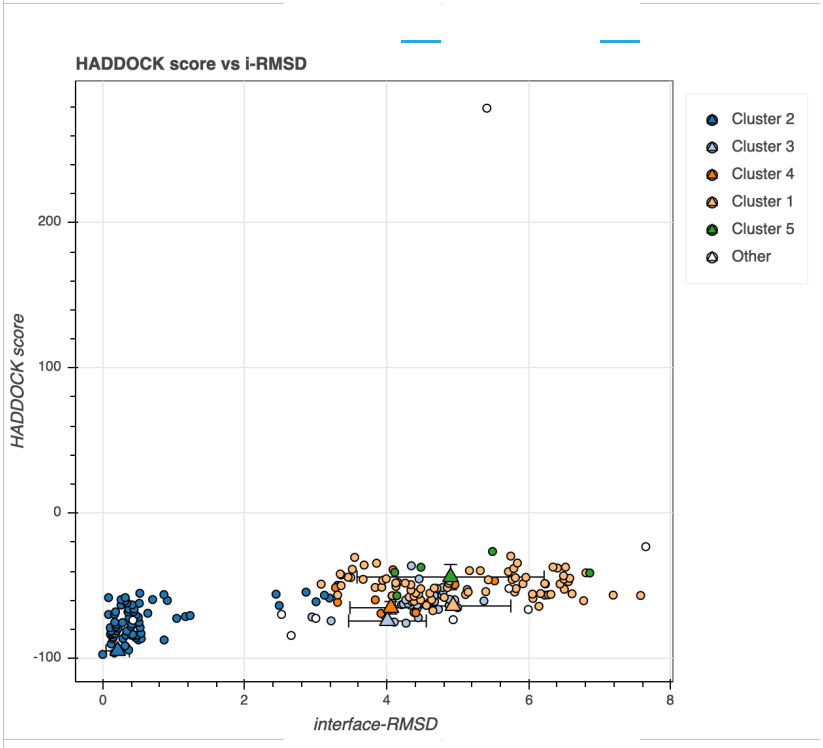
HADDOCK score	-44.0 +/- 7.5
Cluster size	5
RMSD from the overall lowest-energy structure	13.3 +/- 1.1
Van der Waals energy	-52.0 +/- 6.2
Electrostatic energy	-89.5 +/- 19.9
Desolvation energy	-5.4 +/- 3.1
Restraints violation energy	312.4 +/- 34.8
Buried Surface Area	1567.3 +/- 43.3
Z-Score	1.5

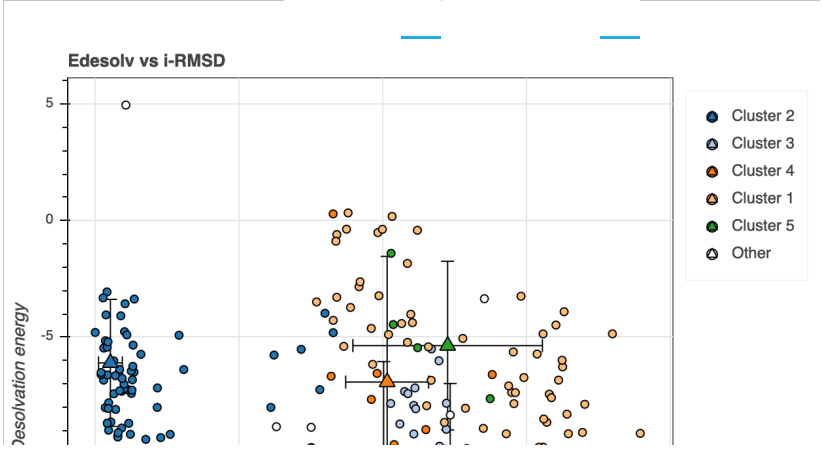
Nr 1 best structure Download file
Nr 2 best structure Download file
Nr 3 best structure Download file
Nr 4 best structure Download file

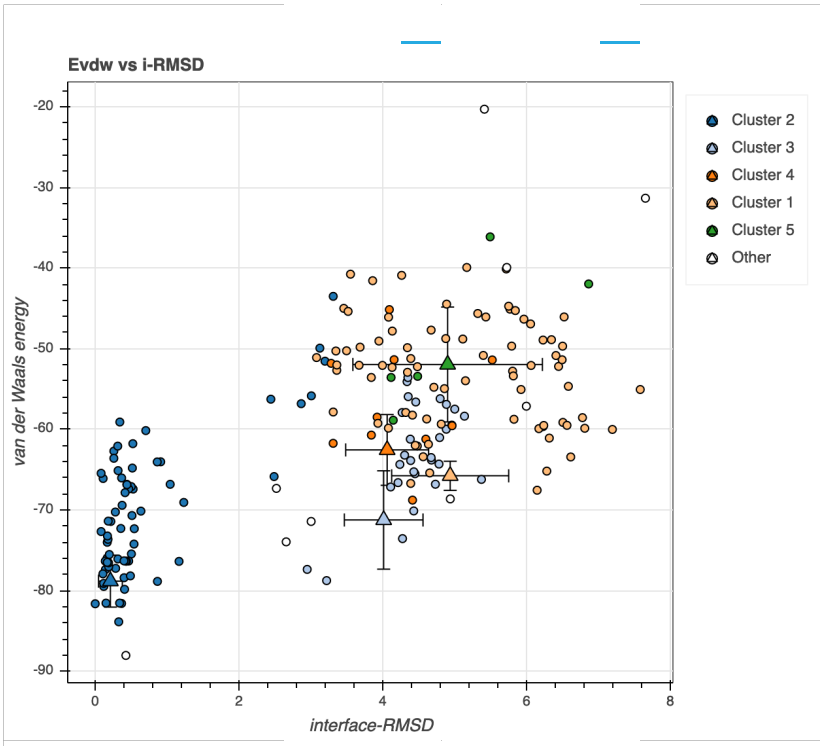
Model Analysis (Download all plots)

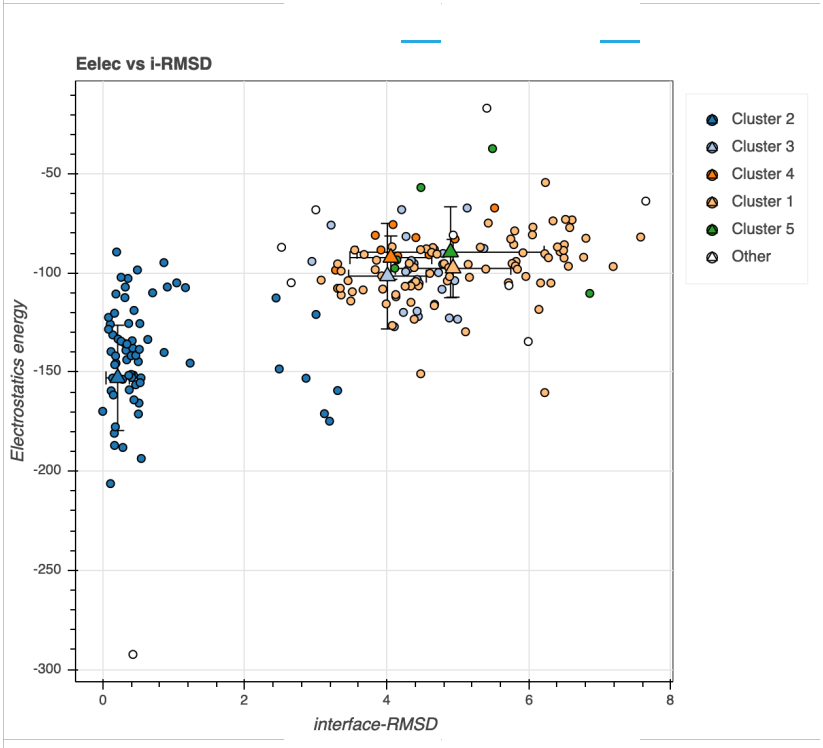
All	None	Cluster 2	Cluster 3	Cluster 4	Cluster 1	Cluster 5	Other

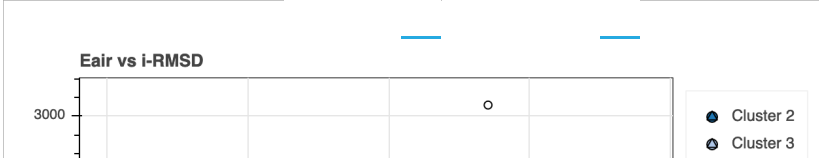

HADDOCK score vs FCC
Cluster 2
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Other
HADDOCK score
200
100
0
-100
0
0.2
0.4
0.6
0.8
1
Fraction of Common Contacts


HADDOCK score vs i-RMSD
Cluster 2
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Other
HADDOCK score
200
100
0
-100
0
2
4
6
8
interface-RMSD


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

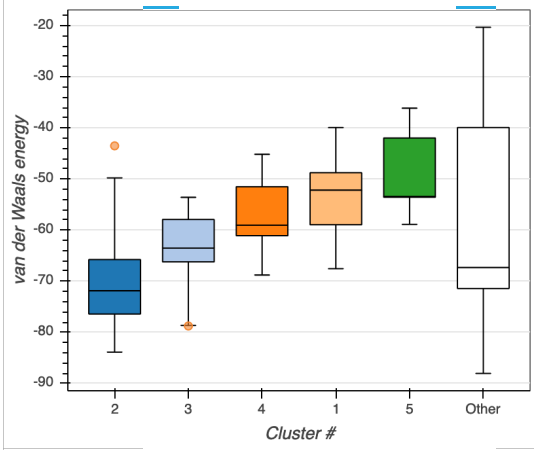

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
Cluster 2
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Other

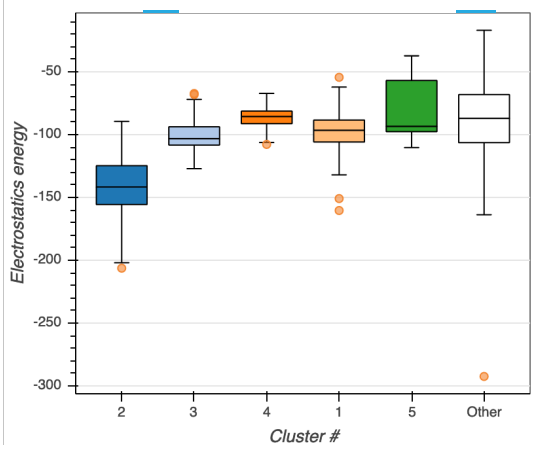

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
Cluster 2
Cluster 3
Cluster 4
Cluster 1
Cluster 5
Other

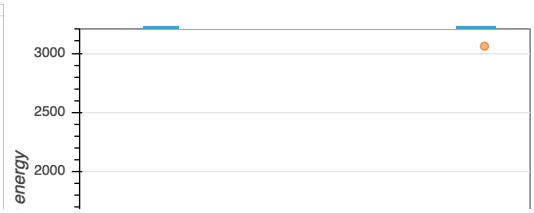

Eair vs i-RMSD
Cluster 2
Cluster 3

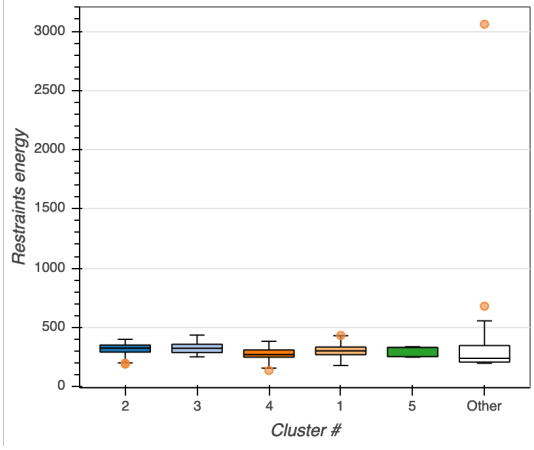
Cluster Analysis

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








Restraints energy
3000
2500
2000
1500
1000
500
0
2
3
4
1
5
Other
Cluster #