HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_TCR-csp-22"

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 **12** 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 2

HADDOCK score	-100.4 +/- 1.5
Cluster size	31
RMSD from the overall lowest-energy structure	16.4 +/- 0.9
Van der Waals energy	-69.6 +/- 6.2
Electrostatic energy	-281.2 +/- 33.9
Desolvation energy	2.7 +/- 3.3
Restraints violation energy	227.2 +/- 35.9
Buried Surface Area	2199.0 +/- 117.4
Z-Score	-1.6

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Nr 3 best structure Download file
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Cluster 1

HADDOCK score	-98.2 +/- 4.8
Cluster size	59
RMSD from the overall lowest-energy structure	0.8 +/- 0.6
Van der Waals energy	-73.3 +/- 4.5
Electrostatic energy	-227.4 +/- 4.1
Desolvation energy	-6.0 +/- 1.5
Restraints violation energy	265.7 +/- 34.6
Buried Surface Area	2080.1 +/- 84.7
Z-Score	-1.4

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Cluster 3

HADDOCK score	-91.6 +/- 5.5
Cluster size	20
RMSD from the overall lowest-energy structure	8.2 +/- 0.5
Van der Waals energy	-71.8 +/- 6.0
Electrostatic energy	-233.6 +/- 19.6
Desolvation energy	0.3 +/- 2.8
Restraints violation energy	265.7 +/- 16.8
Buried Surface Area	2196.8 +/- 86.0

Z-Score	-0.8

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Cluster 9

HADDOCK score	-90.4 +/- 5.8
Cluster size	5
RMSD from the overall lowest-energy structure	8.4 +/- 0.3
Van der Waals energy	-72.3 +/- 6.9
Electrostatic energy	-276.1 +/- 24.4
Desolvation energy	4.2 +/- 1.4
Restraints violation energy	328.9 +/- 65.6
Buried Surface Area	2354.0 +/- 70.6
Z-Score	-0.7

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Cluster 8

HADDOCK score	-86.8 +/- 5.7
Cluster size	5
RMSD from the overall lowest-energy structure	15.3 +/- 0.1
Van der Waals energy	-72.7 +/- 2.1
Electrostatic energy	-196.1 +/- 18.1
Desolvation energy	-0.7 +/- 1.0
Restraints violation energy	258.4 +/- 42.9
Buried Surface Area	2041.0 +/- 46.1
Z-Score	-0.3

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Cluster 10

HADDOCK score	-76.1 +/- 1.2

Cluster size	5
RMSD from the overall lowest-energy structure	14.8 +/- 0.3
Van der Waals energy	-61.2 +/- 7.7
Electrostatic energy	-223.3 +/- 27.4
Desolvation energy	-1.0 +/- 1.5
Restraints violation energy	307.6 +/- 55.8
Buried Surface Area	2094.2 +/- 132.3
Z-Score	0.6

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Cluster 4

HADDOCK score	-74.7 +/- 2.9
Cluster size	15
RMSD from the overall lowest-energy structure	8.9 +/- 0.3
Van der Waals energy	-66.5 +/- 7.4
Electrostatic energy	-137.8 +/- 32.4
Desolvation energy	-6.2 +/- 2.3
Restraints violation energy	256.0 +/- 45.0
Buried Surface Area	2010.9 +/- 84.2
Z-Score	0.8

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Cluster 12

HADDOCK score	-72.5 +/- 11.9
Cluster size	4
RMSD from the overall lowest-energy structure	1.2 +/- 0.9
Van der Waals energy	-59.2 +/- 7.3
Electrostatic energy	-234.4 +/- 9.6
Desolvation energy	-1.1 +/- 4.2
Restraints violation energy	346.7 +/- 78.9
Buried Surface Area	1947.5 +/- 131.7
Z-Score	1.0

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Cluster 7

HADDOCK score	-71.6 +/- 5.3
Cluster size	6
RMSD from the overall lowest-energy structure	19.8 +/- 0.2
Van der Waals energy	-59.5 +/- 4.2
Electrostatic energy	-156.0 +/- 4.7
Desolvation energy	-0.4 +/- 3.5
Restraints violation energy	194.7 +/- 24.8
Buried Surface Area	1940.6 +/- 71.9
Z-Score	1.1

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Cluster 5

HADDOCK score	-69.9 +/- 5.9
Cluster size	13
RMSD from the overall lowest-energy structure	13.6 +/- 0.3
Van der Waals energy	-61.8 +/- 3.9
Electrostatic energy	-157.6 +/- 37.6
Desolvation energy	-4.7 +/- 4.7
Restraints violation energy	280.6 +/- 53.1
Buried Surface Area	1987.3 +/- 122.4
Z-Score	1.2

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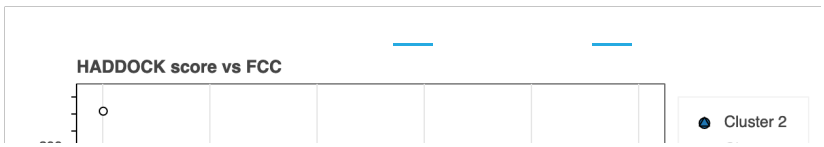
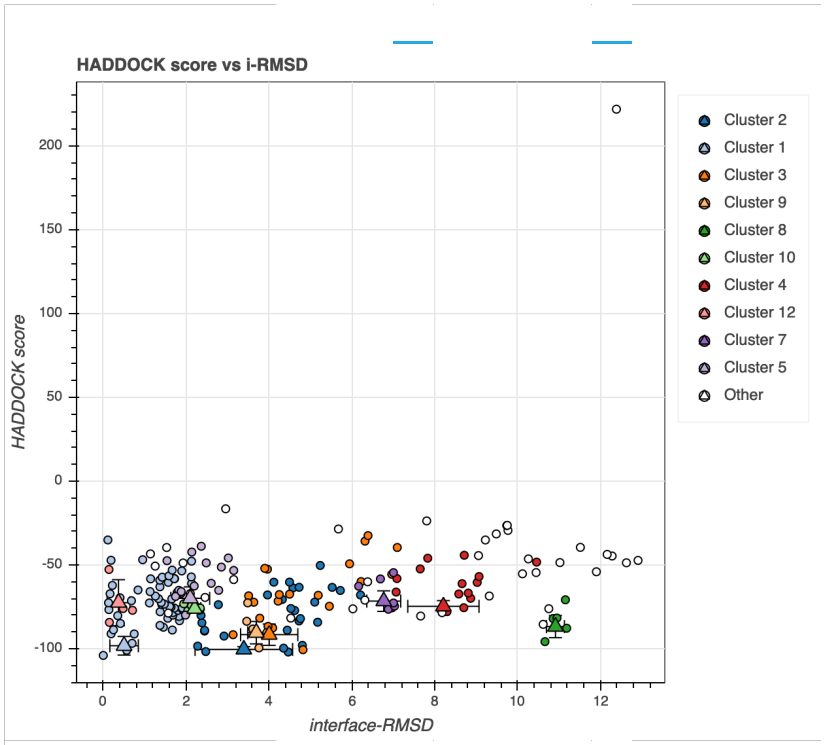
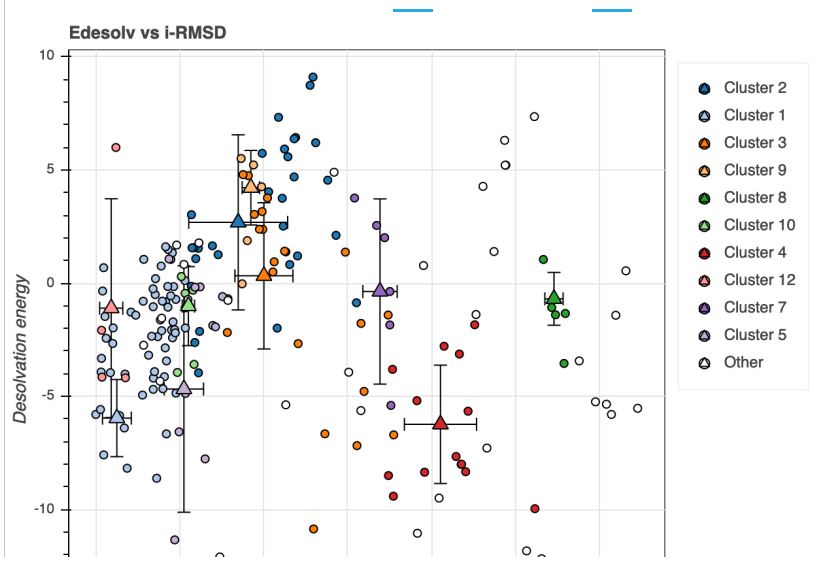
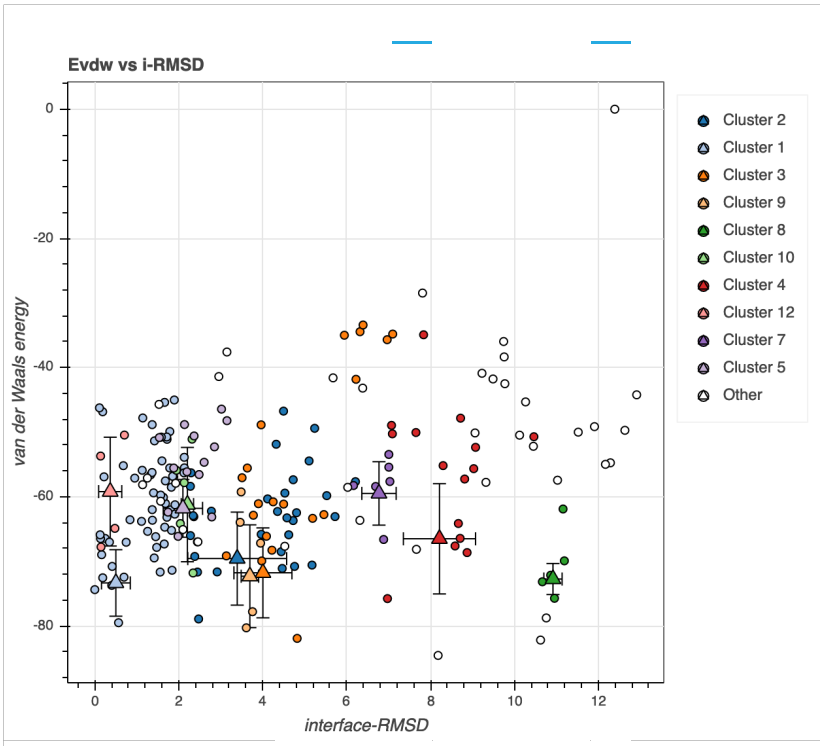
Model Analysis (Download all plots)

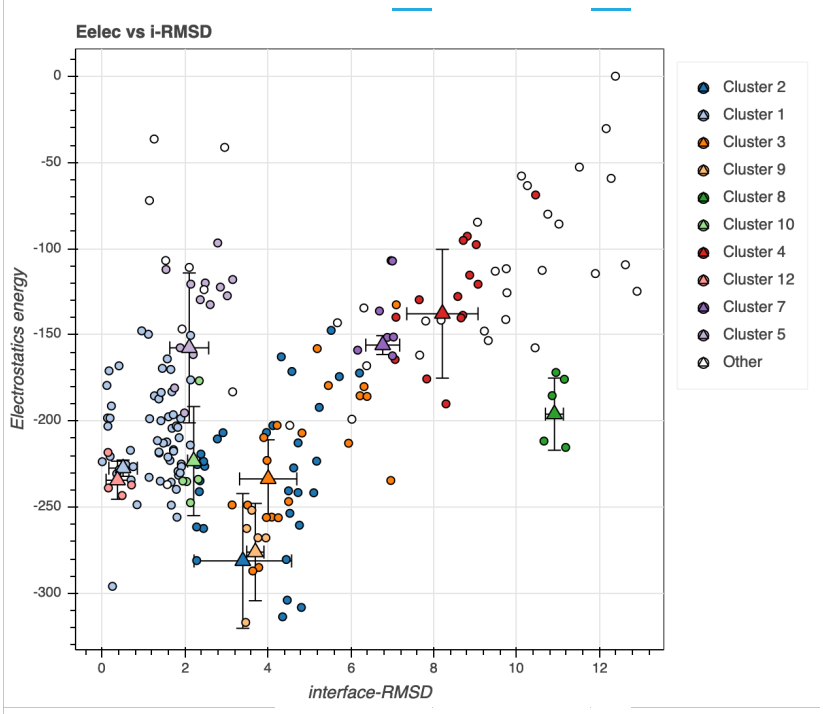
All | None | Cluster 2 | Cluster 1 | Cluster 3 | Cluster 9 | Cluster 8 | Cluster 10 | Cluster 4 | Cluster 12 | Cluster 7 | Cluster 5 | C

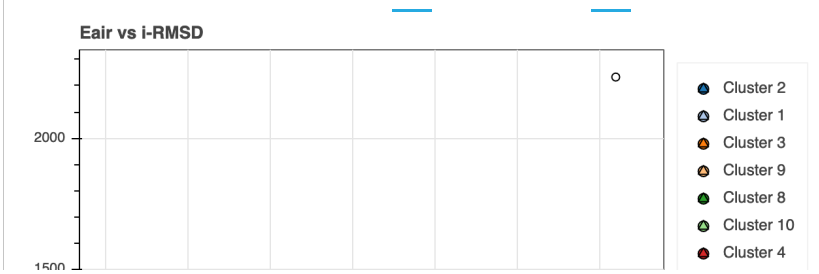



HADDOCK score vs i-RMSD
HADDOCK score
interface-RMSD
200
150
100
50
0
-50
-100
0
2
4
6
8
10
12
Cluster 2
Cluster 1
Cluster 3
Cluster 9
Cluster 8
Cluster 10
Cluster 4
Cluster 12
Cluster 7
Cluster 5
Other


Edesolv vs i-RMSD
Desolvation energy
10
5
0
-5
-10
Cluster 2
Cluster 1
Cluster 3
Cluster 9
Cluster 8
Cluster 10
Cluster 4
Cluster 12
Cluster 7
Cluster 5
Other

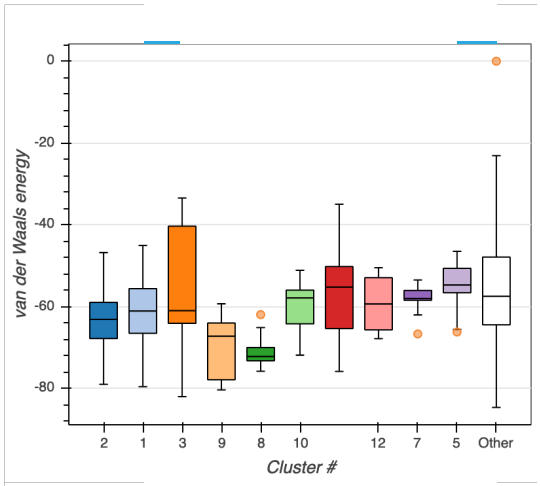

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
0
-20
-40
-60
-80
0
2
4
6
8
10
12
Cluster 2
Cluster 1
Cluster 3
Cluster 9
Cluster 8
Cluster 10
Cluster 4
Cluster 12
Cluster 7
Cluster 5
Other

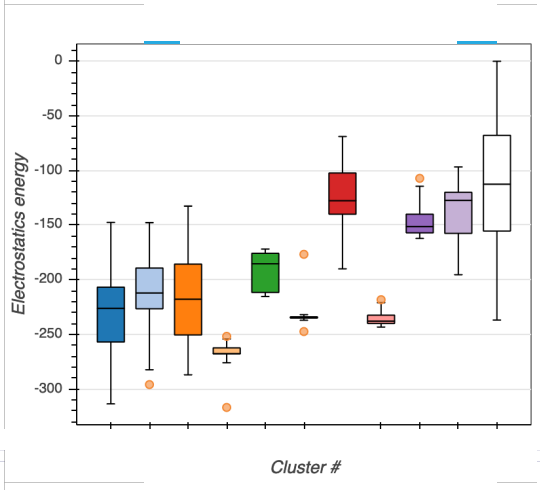

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
0
-50
-100
-150
-200
-250
-300
0
2
4
6
8
10
12
Cluster 2
Cluster 1
Cluster 3
Cluster 9
Cluster 8
Cluster 10
Cluster 4
Cluster 12
Cluster 7
Cluster 5
Other

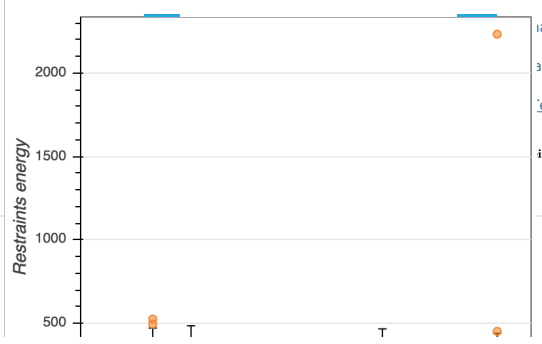

Eair vs i-RMSD
2000
1500
Cluster 2
Cluster 1
Cluster 3
Cluster 9
Cluster 8
Cluster 10
Cluster 4

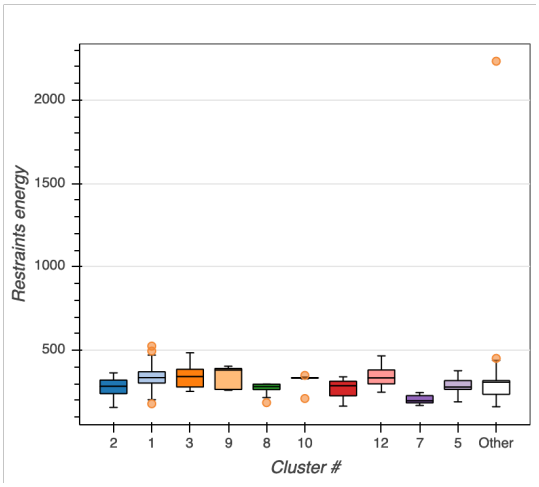
Cluster Analysis

All | None | Cluster 2 | Cluster 1 | Cluster 3 | Cluster 9 | Cluster 8 | Cluster 10 | Cluster 4 | Cluster 12 | Cluster 7 | Cluster 5 | C








Restraints energy
2000
1500
1000
500
2
1
3
9
8
10
12
7
5
Other
Cluster #