HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_TCR-csp-15"

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 **181** structures in **10** cluster(s), which represents **90 %** 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 7

HADDOCK score	-117.4 +/- 4.6
Cluster size	8
RMSD from the overall lowest-energy structure	0.9 +/- 1.0
Van der Waals energy	-69.0 +/- 5.4
Electrostatic energy	-272.1 +/- 42.7
Desolvation energy	-10.3 +/- 3.3
Restraints violation energy	164.0 +/- 45.1
Buried Surface Area	2210.8 +/- 116.1
Z-Score	-1.7

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Cluster 1

HADDOCK score	-110.5 +/- 1.3
Cluster size	50
RMSD from the overall lowest-energy structure	8.9 +/- 0.2
Van der Waals energy	-70.9 +/- 8.8
Electrostatic energy	-283.0 +/- 28.6
Desolvation energy	-4.5 +/- 3.1
Restraints violation energy	215.2 +/- 76.0
Buried Surface Area	2322.1 +/- 71.1
Z-Score	-1.4

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Cluster 5

HADDOCK score	-91.2 +/- 2.9
Cluster size	10
RMSD from the overall lowest-energy structure	4.7 +/- 0.5
Van der Waals energy	-62.7 +/- 6.0
Electrostatic energy	-226.7 +/- 35.7
Desolvation energy	-4.3 +/- 3.4
Restraints violation energy	210.6 +/- 27.5
Buried Surface Area	2113.7 +/- 54.7

Z-Score	-0.4

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Cluster 3

HADDOCK score	-86.1 +/- 2.0
Cluster size	29
RMSD from the overall lowest-energy structure	5.6 +/- 0.8
Van der Waals energy	-71.1 +/- 5.8
Electrostatic energy	-155.8 +/- 28.2
Desolvation energy	-8.7 +/- 4.6
Restraints violation energy	249.2 +/- 38.3
Buried Surface Area	2185.1 +/- 81.6
Z-Score	-0.2

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Cluster 10

HADDOCK score	-82.7 +/- 2.8
Cluster size	4
RMSD from the overall lowest-energy structure	19.1 +/- 0.2
Van der Waals energy	-58.3 +/- 4.8
Electrostatic energy	-219.5 +/- 3.3
Desolvation energy	-10.7 +/- 1.2
Restraints violation energy	302.7 +/- 29.1
Buried Surface Area	2087.2 +/- 53.0
Z-Score	-0.0

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Cluster 2

HADDOCK score	-81.9 +/- 4.1

Cluster size	46
RMSD from the overall lowest-energy structure	17.5 +/- 0.4
Van der Waals energy	-62.1 +/- 1.5
Electrostatic energy	-188.1 +/- 21.9
Desolvation energy	-5.9 +/- 1.9
Restraints violation energy	237.6 +/- 46.0
Buried Surface Area	1914.2 +/- 17.6
Z-Score	0.0

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Cluster 8

HADDOCK score	-81.6 +/- 5.1
Cluster size	7
RMSD from the overall lowest-energy structure	10.1 +/- 0.3
Van der Waals energy	-66.4 +/- 3.3
Electrostatic energy	-196.5 +/- 16.5
Desolvation energy	-7.3 +/- 2.3
Restraints violation energy	314.3 +/- 54.8
Buried Surface Area	1901.8 +/- 59.9
Z-Score	0.0

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Cluster 9

HADDOCK score	-63.3 +/- 8.1
Cluster size	4
RMSD from the overall lowest-energy structure	16.9 +/- 0.6
Van der Waals energy	-50.9 +/- 9.3
Electrostatic energy	-188.6 +/- 22.8
Desolvation energy	-9.7 +/- 2.4
Restraints violation energy	350.5 +/- 10.3
Buried Surface Area	1986.9 +/- 96.3
Z-Score	0.9

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Cluster 4

HADDOCK score	-57.3 +/- 3.4
Cluster size	15
RMSD from the overall lowest-energy structure	18.6 +/- 0.2
Van der Waals energy	-41.2 +/- 6.1
Electrostatic energy	-237.4 +/- 15.6
Desolvation energy	-5.2 +/- 1.3
Restraints violation energy	365.7 +/- 15.9
Buried Surface Area	1634.0 +/- 69.5
Z-Score	1.2

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Cluster 6

HADDOCK score	-48.8 +/- 6.0
Cluster size	8
RMSD from the overall lowest-energy structure	16.4 +/- 0.4
Van der Waals energy	-49.1 +/- 6.2
Electrostatic energy	-126.6 +/- 15.4
Desolvation energy	-10.0 +/- 4.5
Restraints violation energy	357.4 +/- 32.2
Buried Surface Area	1636.6 +/- 82.1
Z-Score	1.6

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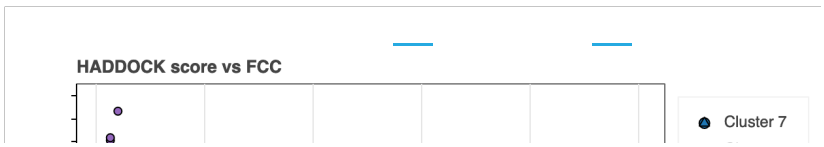
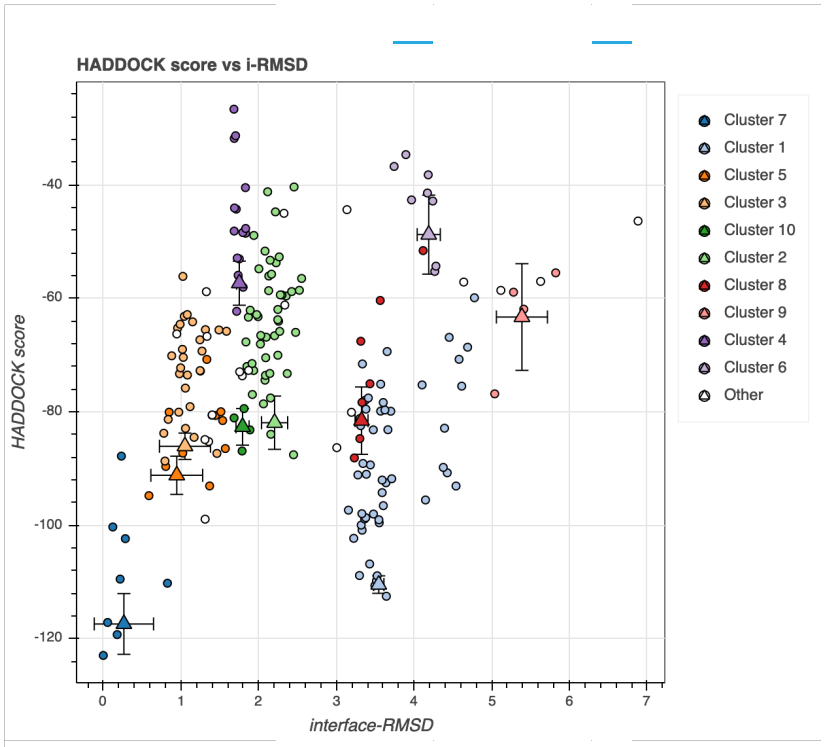
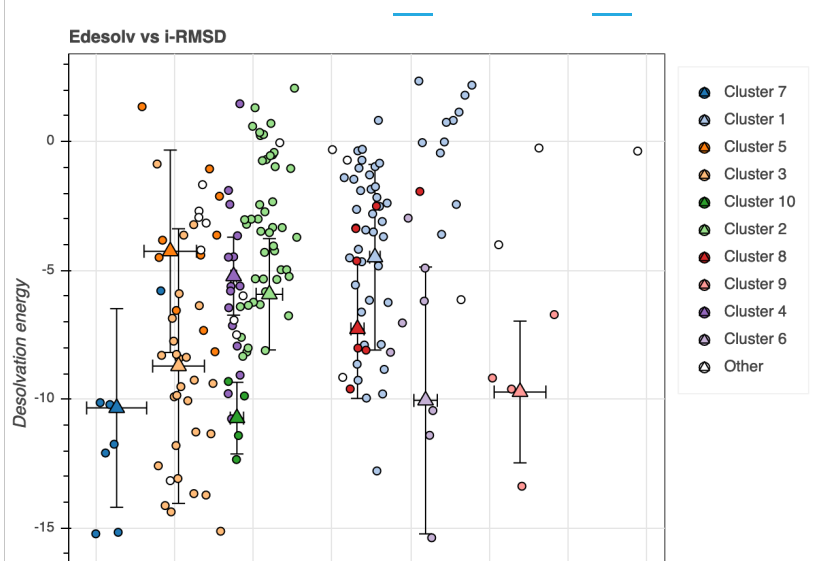
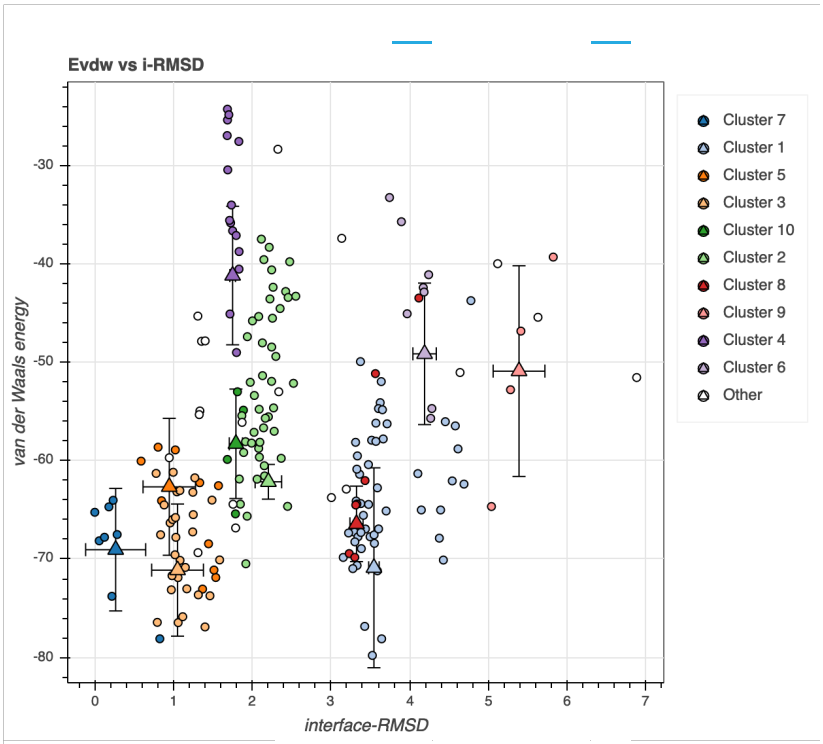
Model Analysis (Download all plots)

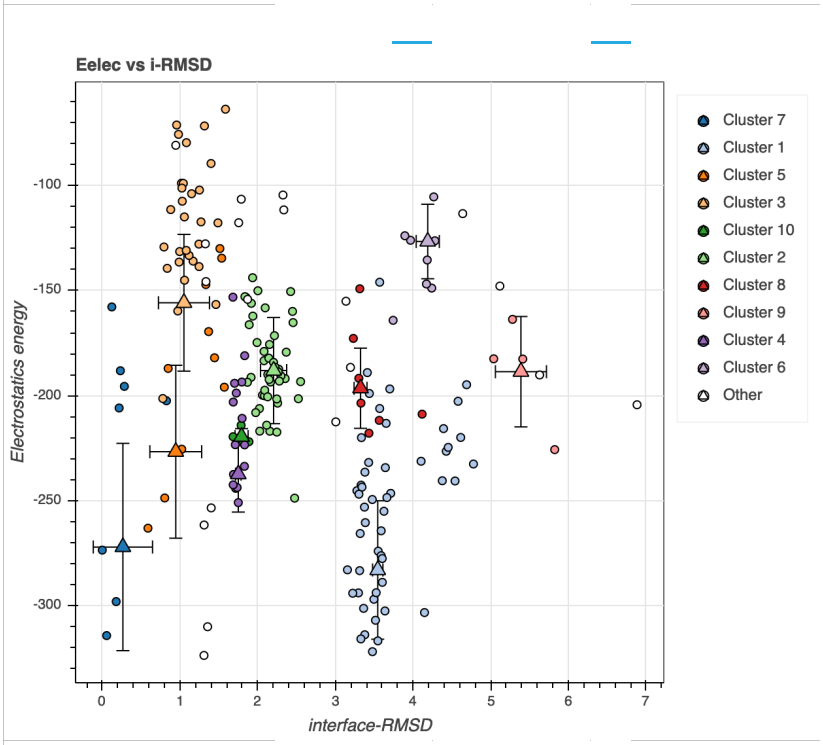
All | None | Cluster 7 | Cluster 1 | Cluster 5 | Cluster 3 | Cluster 10 | Cluster 2 | Cluster 8 | Cluster 9 | Cluster 4 | Cluster 6 | C

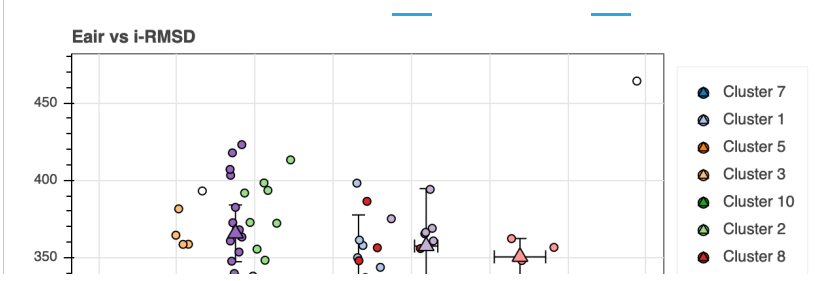



HADDOCK score vs i-RMSD
HADDOCK score
interface-RMSD
-40
-60
-80
-100
-120
0
1
2
3
4
5
6
7
Cluster 7
Cluster 1
Cluster 5
Cluster 3
Cluster 10
Cluster 2
Cluster 8
Cluster 9
Cluster 4
Cluster 6
Other


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

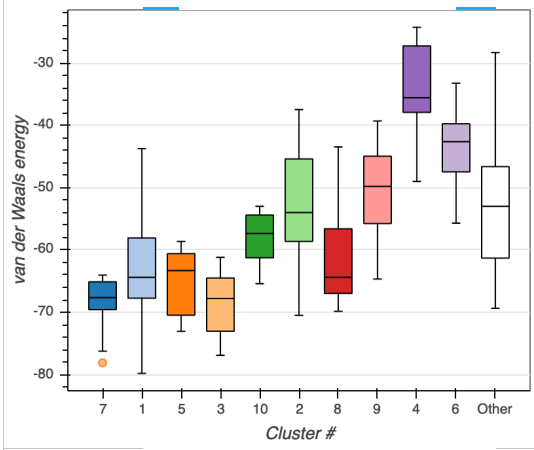

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
-30
-40
-50
-60
-70
-80
0
1
2
3
4
5
6
7
Cluster 7
Cluster 1
Cluster 5
Cluster 3
Cluster 10
Cluster 2
Cluster 8
Cluster 9
Cluster 4
Cluster 6
Other

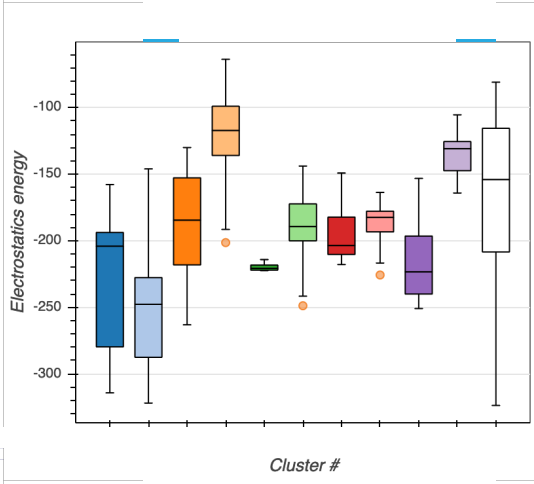

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
-100
-150
-200
-250
-300
0
1
2
3
4
5
6
7
Cluster 7
Cluster 1
Cluster 5
Cluster 3
Cluster 10
Cluster 2
Cluster 8
Cluster 9
Cluster 4
Cluster 6
Other

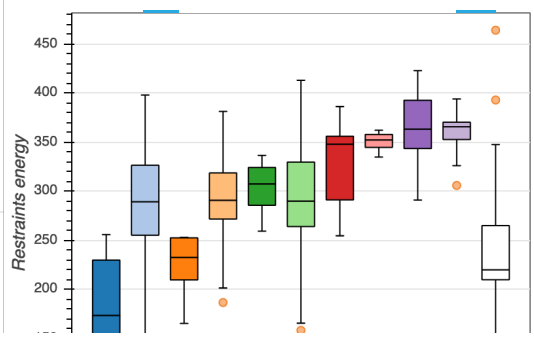

Eair vs i-RMSD
450
400
350
Cluster 7
Cluster 1
Cluster 5
Cluster 3
Cluster 10
Cluster 2
Cluster 8

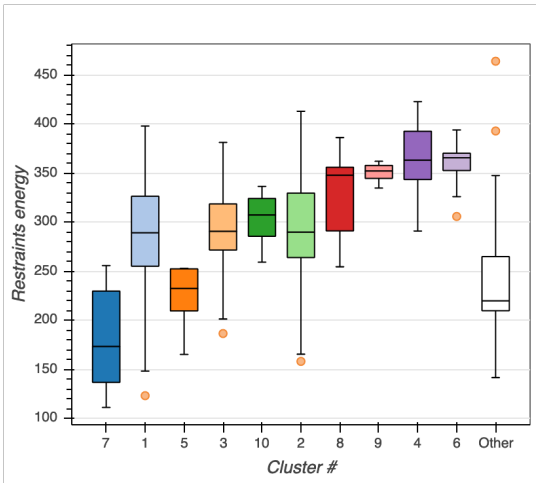
Cluster Analysis

All | None | Cluster 7 | Cluster 1 | Cluster 5 | Cluster 3 | Cluster 10 | Cluster 2 | Cluster 8 | Cluster 9 | Cluster 4 | Cluster 6 | C








Restraints energy
450
400
350
300
250
200
150
100
7
1
5
3
10
2
8
9
4
6
Other
Cluster #