HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_HLA-csp_reference"

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 **163** structures in **10** cluster(s), which represents **81 %** 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	-76.7 +/- 6.7
Cluster size	66
RMSD from the overall lowest-energy structure	0.3 +/- 0.2
Van der Waals energy	-29.7 +/- 7.2
Electrostatic energy	-217.0 +/- 69.8
Desolvation energy	-5.2 +/- 3.5
Restraints violation energy	15.8 +/- 14.4
Buried Surface Area	1173.7 +/- 38.3
Z-Score	-2.2

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

Cluster 4

HADDOCK score	-60.4 +/- 5.9
Cluster size	15
RMSD from the overall lowest-energy structure	0.7 +/- 0.0
Van der Waals energy	-17.3 +/- 3.5
Electrostatic energy	-242.2 +/- 36.4
Desolvation energy	4.5 +/- 1.1
Restraints violation energy	9.1 +/- 12.0
Buried Surface Area	1128.2 +/- 64.6
Z-Score	-0.8

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Cluster 2

HADDOCK score	-60.0 +/- 7.7
Cluster size	24
RMSD from the overall lowest-energy structure	0.5 +/- 0.1
Van der Waals energy	-19.7 +/- 7.2
Electrostatic energy	-184.1 +/- 77.8
Desolvation energy	-4.4 +/- 3.6
Restraints violation energy	9.0 +/- 3.9
Buried Surface Area	1022.0 +/- 51.8

Z-Score	-0.8

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Cluster 3

HADDOCK score	-53.9 +/- 4.2
Cluster size	23
RMSD from the overall lowest-energy structure	1.4 +/- 0.1
Van der Waals energy	-20.6 +/- 2.2
Electrostatic energy	-167.6 +/- 6.5
Desolvation energy	-3.0 +/- 1.9
Restraints violation energy	32.3 +/- 19.6
Buried Surface Area	851.9 +/- 47.0
Z-Score	-0.3

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Cluster 10

HADDOCK score	-47.7 +/- 6.5
Cluster size	4
RMSD from the overall lowest-energy structure	1.6 +/- 0.1
Van der Waals energy	-20.1 +/- 8.7
Electrostatic energy	-122.2 +/- 50.5
Desolvation energy	-5.7 +/- 0.9
Restraints violation energy	25.4 +/- 15.1
Buried Surface Area	971.3 +/- 95.0
Z-Score	0.2

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Cluster 6

HADDOCK score	-44.3 +/- 1.9

Cluster size	8
RMSD from the overall lowest-energy structure	1.4 +/- 0.1
Van der Waals energy	-17.9 +/- 5.8
Electrostatic energy	-134.4 +/- 27.5
Desolvation energy	-2.3 +/- 1.0
Restraints violation energy	29.0 +/- 12.0
Buried Surface Area	898.2 +/- 51.0
Z-Score	0.5

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Nr 4 best structure Download file

Cluster 5

HADDOCK score	-44.0 +/- 1.8
Cluster size	9
RMSD from the overall lowest-energy structure	0.6 +/- 0.1
Van der Waals energy	-9.3 +/- 7.1
Electrostatic energy	-156.0 +/- 63.3
Desolvation energy	-3.8 +/- 5.9
Restraints violation energy	2.9 +/- 1.7
Buried Surface Area	788.7 +/- 71.7
Z-Score	0.5

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Nr 3 best structure Download file
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Cluster 8

HADDOCK score	-43.2 +/- 1.2
Cluster size	5
RMSD from the overall lowest-energy structure	0.9 +/- 0.1
Van der Waals energy	-17.5 +/- 4.9
Electrostatic energy	-123.2 +/- 28.5
Desolvation energy	-3.1 +/- 1.1
Restraints violation energy	20.8 +/- 15.3
Buried Surface Area	863.3 +/- 16.6
Z-Score	0.6

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Cluster 7

HADDOCK score	-36.8 +/- 4.1
Cluster size	5
RMSD from the overall lowest-energy structure	1.5 +/- 0.1
Van der Waals energy	-14.8 +/- 6.0
Electrostatic energy	-113.6 +/- 49.0
Desolvation energy	-0.6 +/- 3.1
Restraints violation energy	14.0 +/- 12.3
Buried Surface Area	792.1 +/- 90.9
Z-Score	1.1

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Cluster 9

HADDOCK score	-35.6 +/- 2.8
Cluster size	4
RMSD from the overall lowest-energy structure	1.1 +/- 0.2
Van der Waals energy	-15.3 +/- 2.8
Electrostatic energy	-104.5 +/- 10.0
Desolvation energy	-1.6 +/- 0.7
Restraints violation energy	22.2 +/- 21.2
Buried Surface Area	743.6 +/- 54.9
Z-Score	1.2

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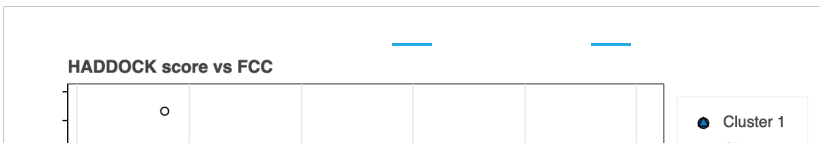
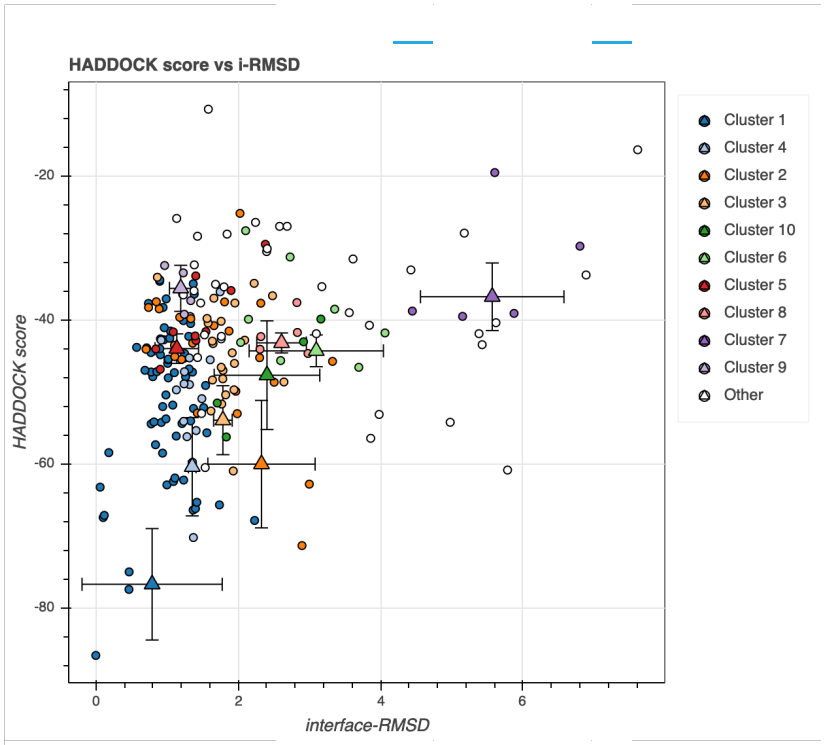
Nr 3 best structure Download file

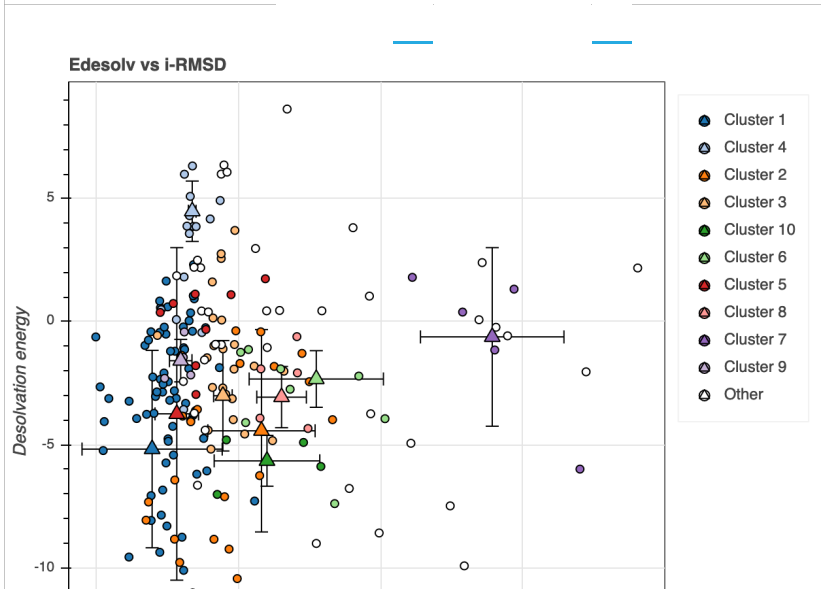
Nr 4 best structure Download file

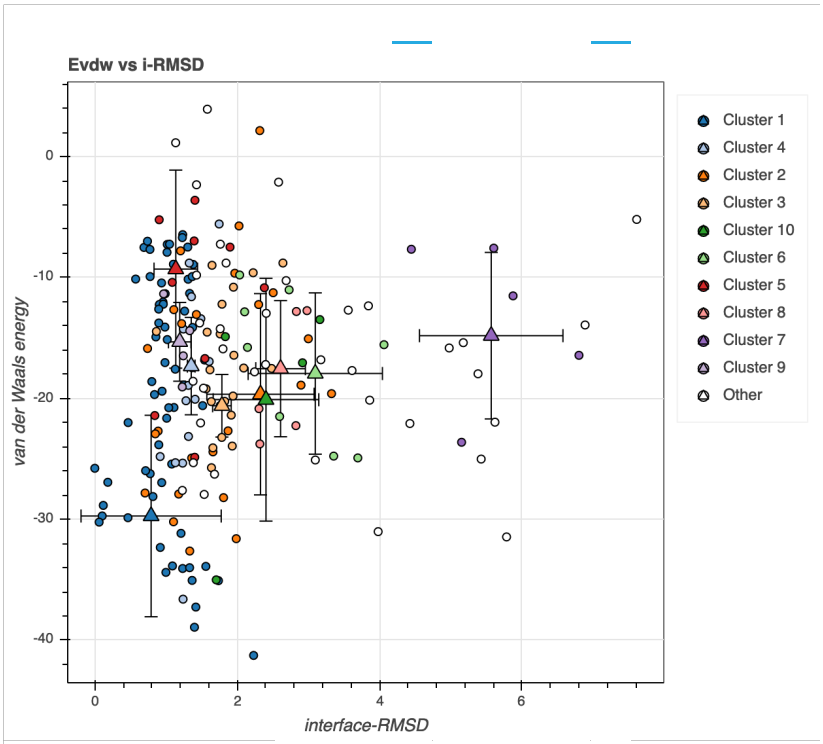
Model Analysis (Download all plots)

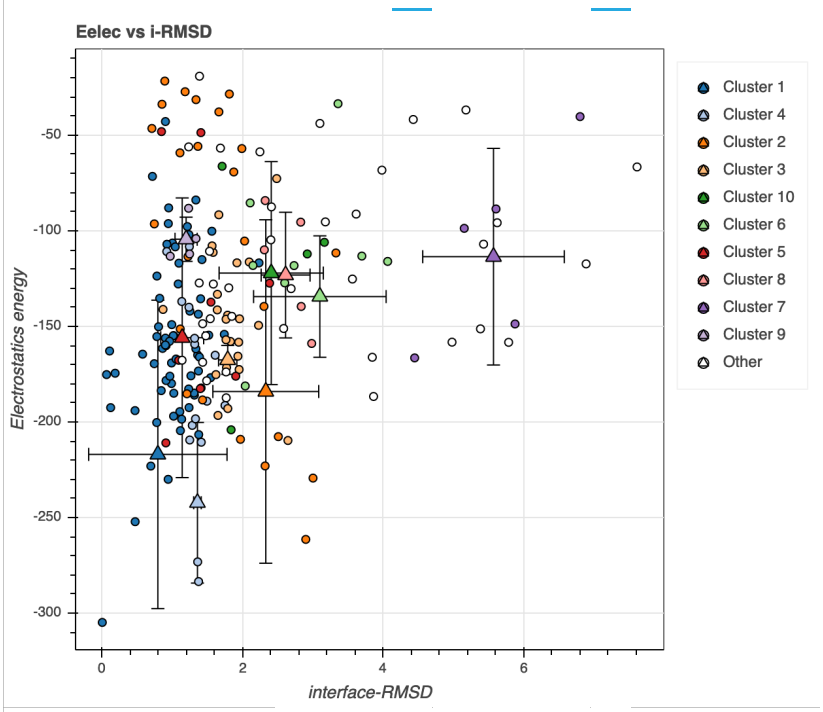
All | None | Cluster 1 | Cluster 4 | Cluster 2 | Cluster 3 | Cluster 10 | Cluster 6 | Cluster 5 | Cluster 8 | Cluster 7 | Cluster 9 | C

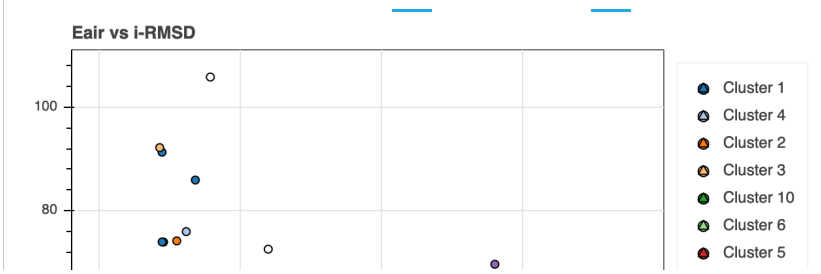



HADDOCK score vs i-RMSD
HADDOCK score
interface-RMSD
-20
-40
-60
-80
0
2
4
6
Cluster 1
Cluster 4
Cluster 2
Cluster 3
Cluster 10
Cluster 6
Cluster 5
Cluster 8
Cluster 7
Cluster 9
Other


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

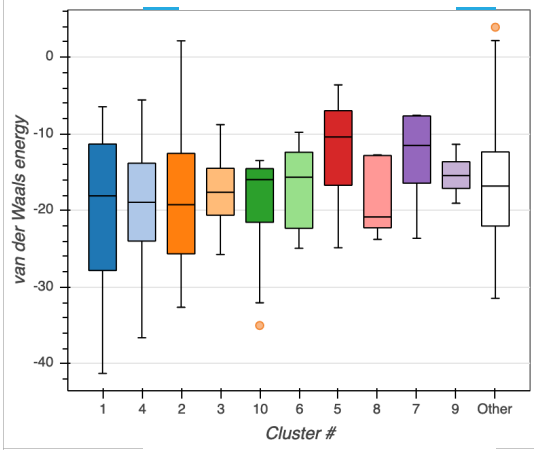

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
0
-10
-20
-30
-40
0
2
4
6
Cluster 1
Cluster 4
Cluster 2
Cluster 3
Cluster 10
Cluster 6
Cluster 5
Cluster 8
Cluster 7
Cluster 9
Other

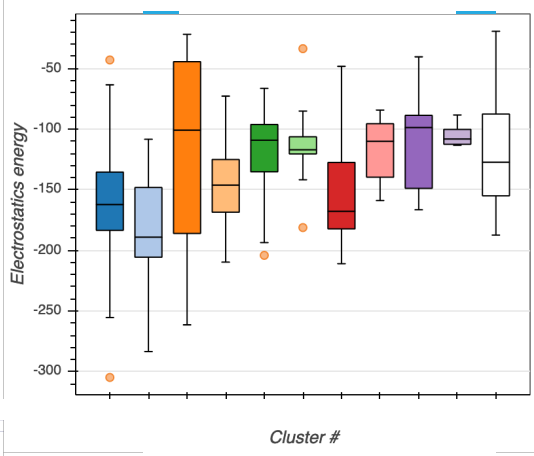

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
-50
-100
-150
-200
-250
-300
0
2
4
6
Cluster 1
Cluster 4
Cluster 2
Cluster 3
Cluster 10
Cluster 6
Cluster 5
Cluster 8
Cluster 7
Cluster 9
Other

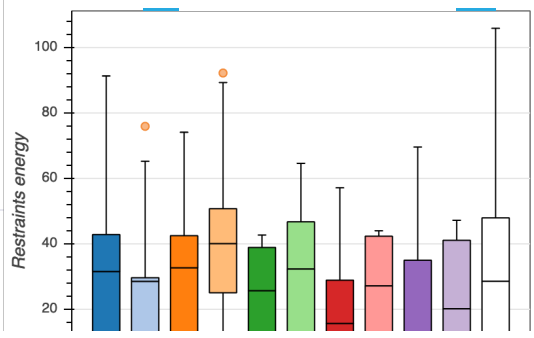

Eair vs i-RMSD
100
80
Cluster 1
Cluster 4
Cluster 2
Cluster 3
Cluster 10
Cluster 6
Cluster 5

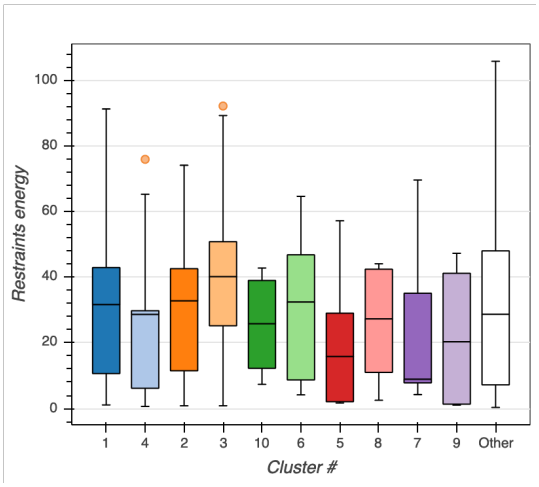
Cluster Analysis

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








Restraints energy
100
80
60
40
20
0
1
4
2
3
10
6
5
8
7
9
Other
Cluster #