HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_TCR-csp-4"

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 **168** structures in **10** cluster(s), which represents **84 %** 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	-99.6 +/- 5.1
Cluster size	6
RMSD from the overall lowest-energy structure	0.5 +/- 0.3
Van der Waals energy	-65.3 +/- 3.1
Electrostatic energy	-274.9 +/- 35.4
Desolvation energy	0.5 +/- 4.8
Restraints violation energy	201.9 +/- 40.9
Buried Surface Area	2135.9 +/- 41.5
Z-Score	-1.2

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Cluster 2

HADDOCK score	-95.1 +/- 5.8
Cluster size	35
RMSD from the overall lowest-energy structure	21.1 +/- 0.1
Van der Waals energy	-64.7 +/- 3.9
Electrostatic energy	-243.3 +/- 24.6
Desolvation energy	-3.7 +/- 2.0
Restraints violation energy	219.2 +/- 28.3
Buried Surface Area	2268.9 +/- 79.1
Z-Score	-1.0

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Cluster 1

HADDOCK score	-94.3 +/- 1.2
Cluster size	37
RMSD from the overall lowest-energy structure	10.9 +/- 0.3
Van der Waals energy	-73.6 +/- 6.0
Electrostatic energy	-195.6 +/- 42.3
Desolvation energy	-0.7 +/- 1.2
Restraints violation energy	191.2 +/- 25.2
Buried Surface Area	2080.1 +/- 58.6

Z-Score	-1.0

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Cluster 3

HADDOCK score	-92.3 +/- 7.2
Cluster size	24
RMSD from the overall lowest-energy structure	8.3 +/- 0.2
Van der Waals energy	-75.7 +/- 5.0
Electrostatic energy	-171.9 +/- 21.9
Desolvation energy	-10.0 +/- 1.5
Restraints violation energy	277.6 +/- 71.2
Buried Surface Area	2047.3 +/- 120.5
Z-Score	-0.9

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Cluster 4

HADDOCK score	-89.0 +/- 7.1
Cluster size	22
RMSD from the overall lowest-energy structure	14.7 +/- 0.8
Van der Waals energy	-72.3 +/- 2.5
Electrostatic energy	-171.1 +/- 46.5
Desolvation energy	-2.7 +/- 2.4
Restraints violation energy	202.8 +/- 8.7
Buried Surface Area	2006.5 +/- 116.4
Z-Score	-0.7

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Cluster 10

HADDOCK score	-66.3 +/- 4.3

Cluster size	4
RMSD from the overall lowest-energy structure	7.8 +/- 0.2
Van der Waals energy	-61.2 +/- 2.7
Electrostatic energy	-145.3 +/- 23.9
Desolvation energy	-9.1 +/- 2.0
Restraints violation energy	330.1 +/- 67.1
Buried Surface Area	1929.8 +/- 80.6
Z-Score	0.4

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Cluster 6

HADDOCK score	-60.1 +/- 4.9
Cluster size	13
RMSD from the overall lowest-energy structure	20.4 +/- 0.2
Van der Waals energy	-61.6 +/- 4.7
Electrostatic energy	-106.9 +/- 26.1
Desolvation energy	-4.7 +/- 3.1
Restraints violation energy	276.1 +/- 47.0
Buried Surface Area	1922.5 +/- 130.1
Z-Score	0.7

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Cluster 5

HADDOCK score	-55.1 +/- 1.0
Cluster size	19
RMSD from the overall lowest-energy structure	21.6 +/- 0.3
Van der Waals energy	-48.6 +/- 6.2
Electrostatic energy	-136.1 +/- 44.1
Desolvation energy	-4.0 +/- 2.5
Restraints violation energy	246.5 +/- 48.2
Buried Surface Area	1560.0 +/- 115.7
Z-Score	1.0

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Cluster 9

HADDOCK score	-48.5 +/- 5.8
Cluster size	4
RMSD from the overall lowest-energy structure	11.5 +/- 0.3
Van der Waals energy	-43.8 +/- 3.1
Electrostatic energy	-144.2 +/- 17.7
Desolvation energy	-6.4 +/- 2.4
Restraints violation energy	304.4 +/- 53.2
Buried Surface Area	1351.2 +/- 41.1
Z-Score	1.3

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Cluster 8

HADDOCK score	-45.5 +/- 4.9
Cluster size	4
RMSD from the overall lowest-energy structure	16.8 +/- 0.5
Van der Waals energy	-48.9 +/- 1.9
Electrostatic energy	-106.3 +/- 15.7
Desolvation energy	-4.9 +/- 0.7
Restraints violation energy	294.8 +/- 17.7
Buried Surface Area	1479.9 +/- 67.4
Z-Score	1.4

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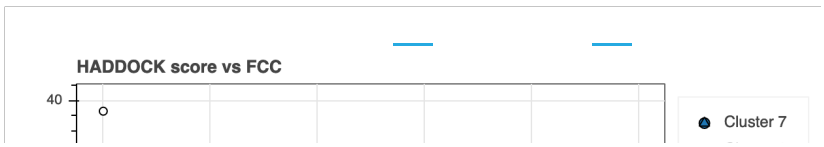
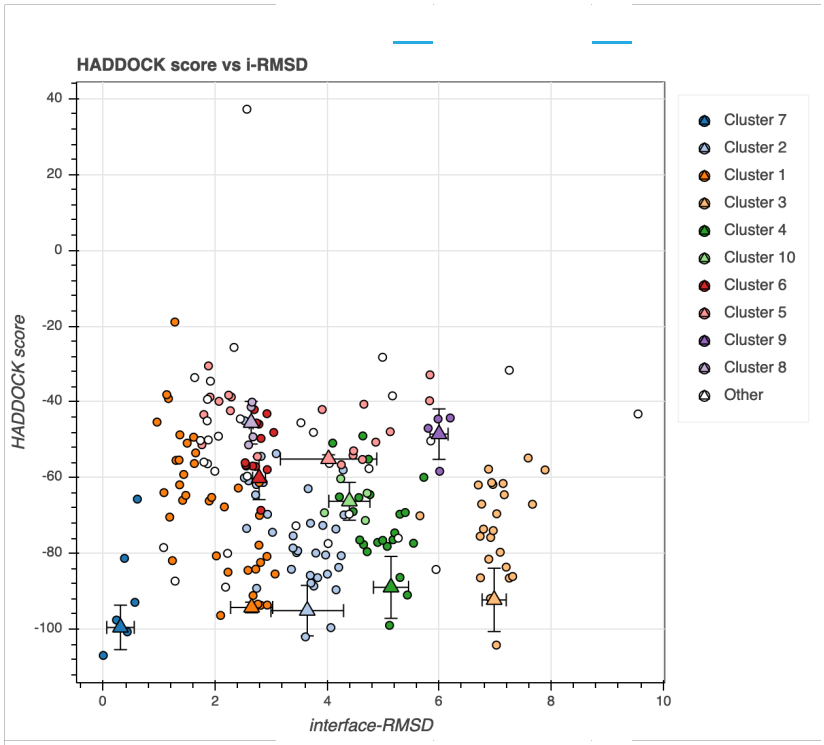
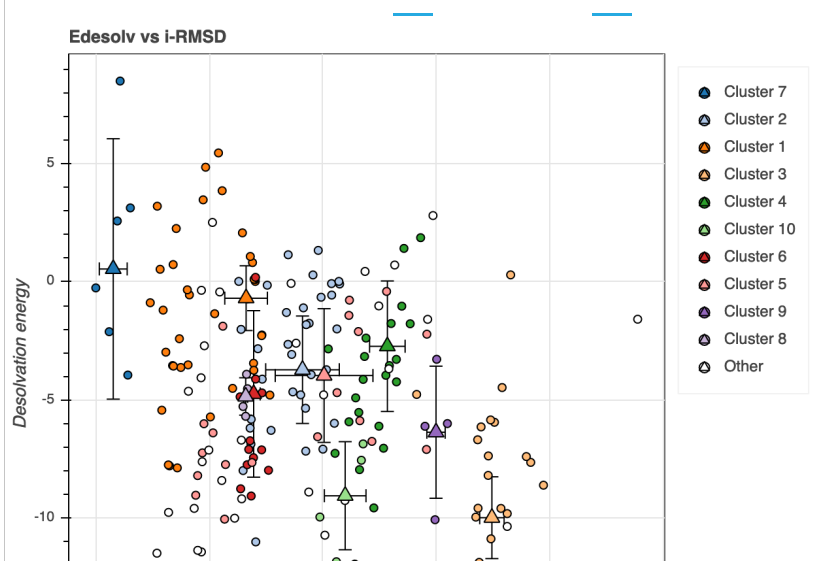
Nr 4 best structure Download file

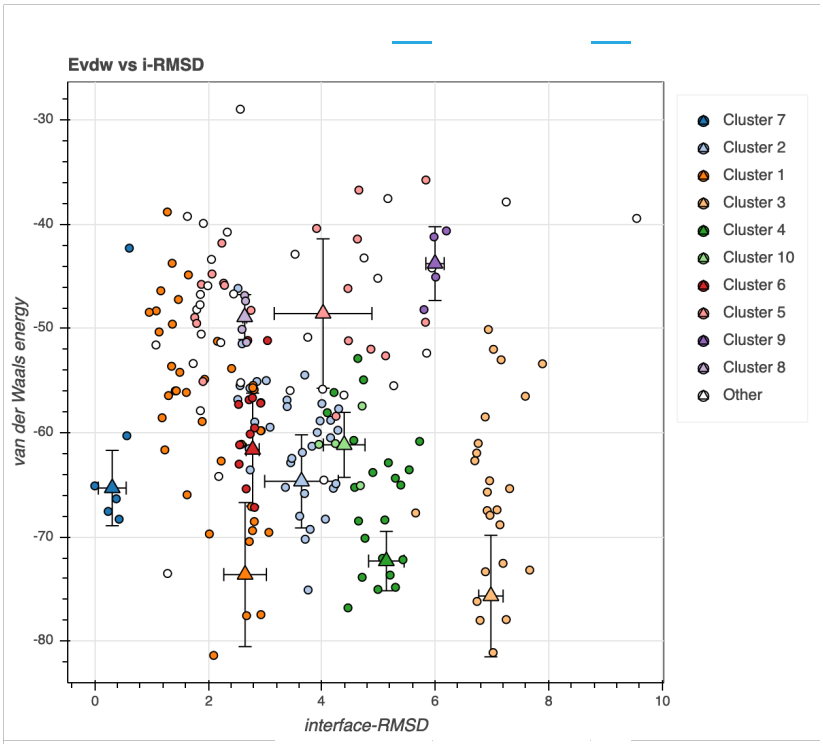
Model Analysis (Download all plots)

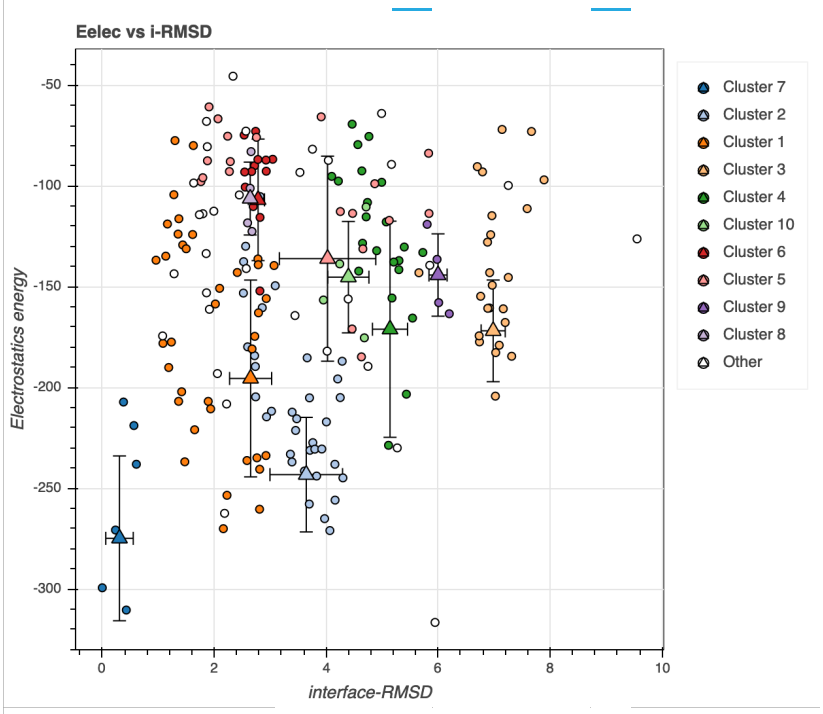
All | None | Cluster 7 | Cluster 2 | Cluster 1 | Cluster 3 | Cluster 4 | Cluster 10 | Cluster 6 | Cluster 5 | Cluster 9 | Cluster 8 | C

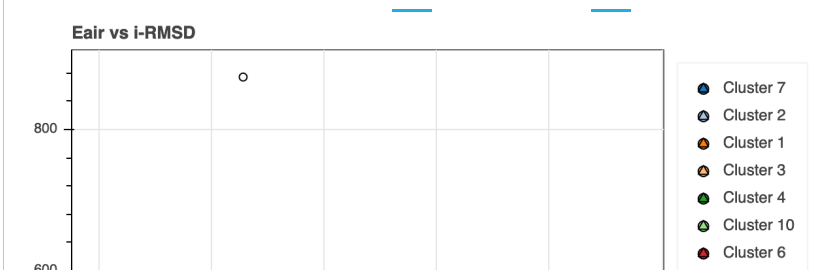



HADDOCK score vs i-RMSD
HADDOCK score
interface-RMSD
Cluster 7
Cluster 2
Cluster 1
Cluster 3
Cluster 4
Cluster 10
Cluster 6
Cluster 5
Cluster 9
Cluster 8
Other


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

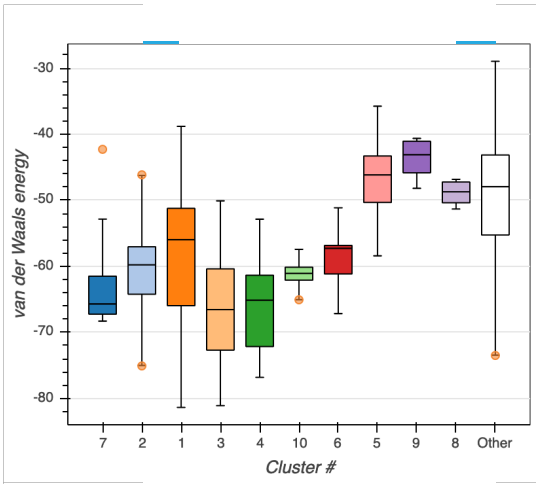

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
-30
-40
-50
-60
-70
-80
0
2
4
6
8
10
Cluster 7
Cluster 2
Cluster 1
Cluster 3
Cluster 4
Cluster 10
Cluster 6
Cluster 5
Cluster 9
Cluster 8
Other

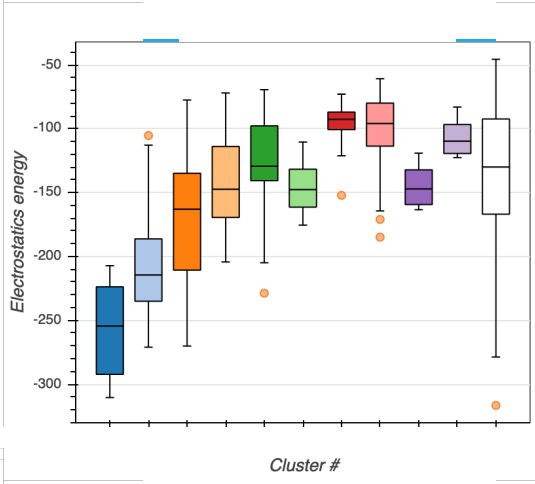

Eelec vs i-RMSD
Electrostatics energy
interface-RMSD
-50
-100
-150
-200
-250
-300
0
2
4
6
8
10
Cluster 7
Cluster 2
Cluster 1
Cluster 3
Cluster 4
Cluster 10
Cluster 6
Cluster 5
Cluster 9
Cluster 8
Other

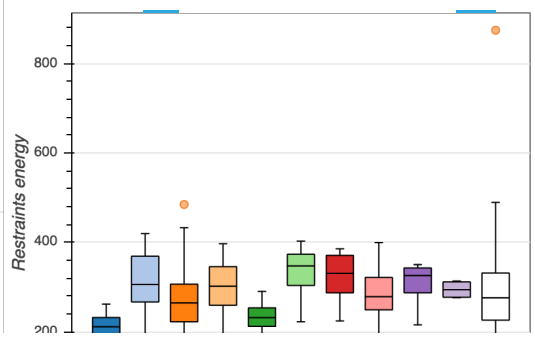

Eair vs i-RMSD
800
Cluster 7
Cluster 2
Cluster 1
Cluster 3
Cluster 4
Cluster 10
Cluster 6

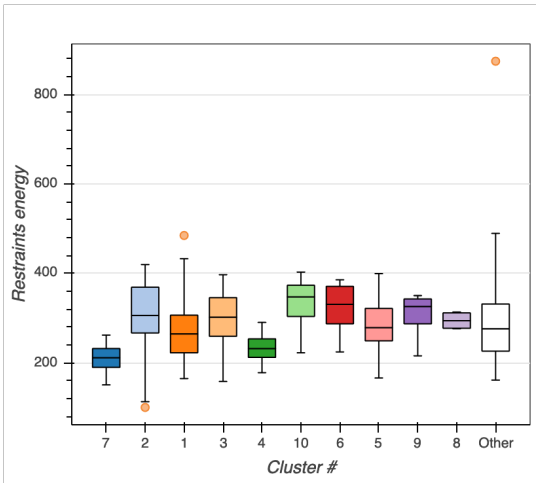
Cluster Analysis

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








Restraints energy
800
600
400
200
7
2
1
3
4
10
6
5
9
8
Other
Cluster #