HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_TCR-csp-117"

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 **183** structures in **9** cluster(s), which represents **91 %** 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 3

HADDOCK score	-118.5 +/- 1.8
Cluster size	11
RMSD from the overall lowest-energy structure	4.0 +/- 0.2
Van der Waals energy	-64.6 +/- 3.1
Electrostatic energy	-378.6 +/- 12.9
Desolvation energy	2.4 +/- 1.9
Restraints violation energy	194.6 +/- 20.1
Buried Surface Area	2013.1 +/- 33.7
Z-Score	-1.8

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Cluster 1

HADDOCK score	-110.3 +/- 1.0
Cluster size	102
RMSD from the overall lowest-energy structure	9.1 +/- 0.1
Van der Waals energy	-81.0 +/- 2.5
Electrostatic energy	-250.2 +/- 18.1
Desolvation energy	-2.0 +/- 1.0
Restraints violation energy	228.5 +/- 34.8
Buried Surface Area	2166.8 +/- 81.5
Z-Score	-1.3

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Cluster 2

HADDOCK score	-94.1 +/- 1.8
Cluster size	30
RMSD from the overall lowest-energy structure	21.0 +/- 0.9
Van der Waals energy	-60.6 +/- 3.6
Electrostatic energy	-265.3 +/- 33.6
Desolvation energy	-5.5 +/- 5.0
Restraints violation energy	250.9 +/- 53.5
Buried Surface Area	1780.1 +/- 25.8

Z-Score	-0.5

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Cluster 7

HADDOCK score	-90.0 +/- 24.5
Cluster size	6
RMSD from the overall lowest-energy structure	1.2 +/- 1.0
Van der Waals energy	-60.1 +/- 13.8
Electrostatic energy	-221.2 +/- 41.3
Desolvation energy	-6.0 +/- 0.4
Restraints violation energy	203.0 +/- 40.3
Buried Surface Area	1860.9 +/- 191.2
Z-Score	-0.3

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Cluster 9

HADDOCK score	-82.8 +/- 20.3
Cluster size	4
RMSD from the overall lowest-energy structure	7.1 +/- 1.0
Van der Waals energy	-63.6 +/- 11.3
Electrostatic energy	-199.1 +/- 23.5
Desolvation energy	-0.6 +/- 1.4
Restraints violation energy	212.6 +/- 79.2
Buried Surface Area	1910.0 +/- 72.3
Z-Score	0.1

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Cluster 5

HADDOCK score	-72.6 +/- 7.0

Cluster size	8
RMSD from the overall lowest-energy structure	10.5 +/- 0.1
Van der Waals energy	-49.0 +/- 1.6
Electrostatic energy	-191.6 +/- 21.9
Desolvation energy	-5.5 +/- 2.0
Restraints violation energy	202.1 +/- 44.6
Buried Surface Area	1899.4 +/- 89.2
Z-Score	0.7

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Cluster 4

HADDOCK score	-70.5 +/- 10.9
Cluster size	10
RMSD from the overall lowest-energy structure	18.1 +/- 0.2
Van der Waals energy	-47.1 +/- 4.0
Electrostatic energy	-201.7 +/- 18.2
Desolvation energy	-7.6 +/- 2.2
Restraints violation energy	246.5 +/- 51.6
Buried Surface Area	1738.3 +/- 64.1
Z-Score	0.8

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Cluster 8

HADDOCK score	-69.6 +/- 15.8
Cluster size	5
RMSD from the overall lowest-energy structure	8.2 +/- 0.3
Van der Waals energy	-67.3 +/- 8.4
Electrostatic energy	-86.9 +/- 32.8
Desolvation energy	-11.4 +/- 2.1
Restraints violation energy	264.5 +/- 39.5
Buried Surface Area	2002.9 +/- 114.5
Z-Score	0.8

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Cluster 6

HADDOCK score	-58.3 +/- 9.6
Cluster size	7
RMSD from the overall lowest-energy structure	19.0 +/- 0.4
Van der Waals energy	-48.9 +/- 2.8
Electrostatic energy	-167.5 +/- 35.4
Desolvation energy	-2.3 +/- 3.0
Restraints violation energy	263.6 +/- 34.2
Buried Surface Area	1617.6 +/- 97.1
Z-Score	1.4

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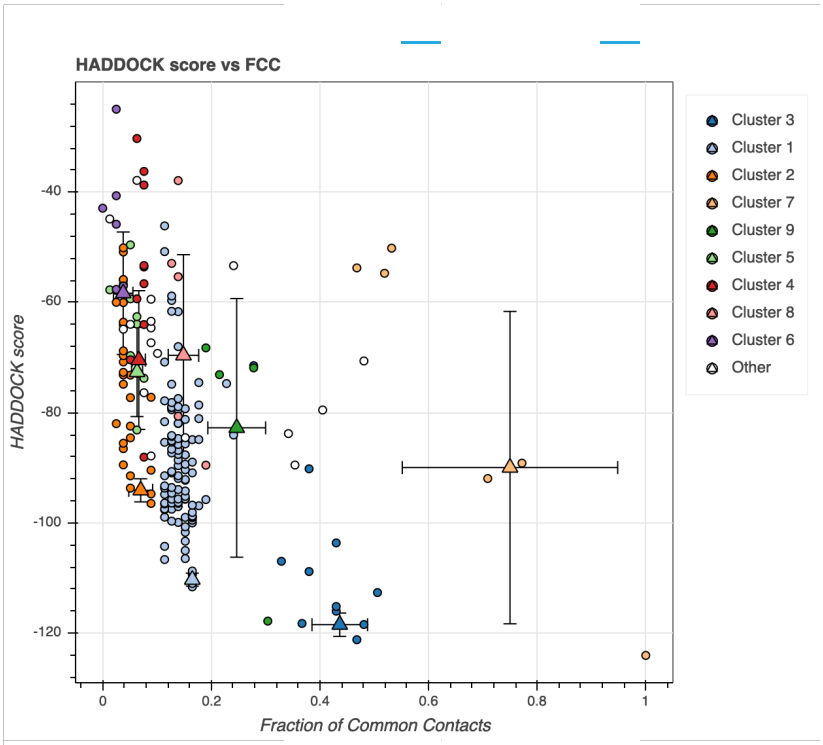
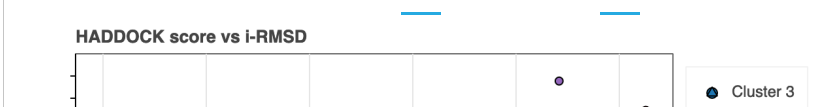
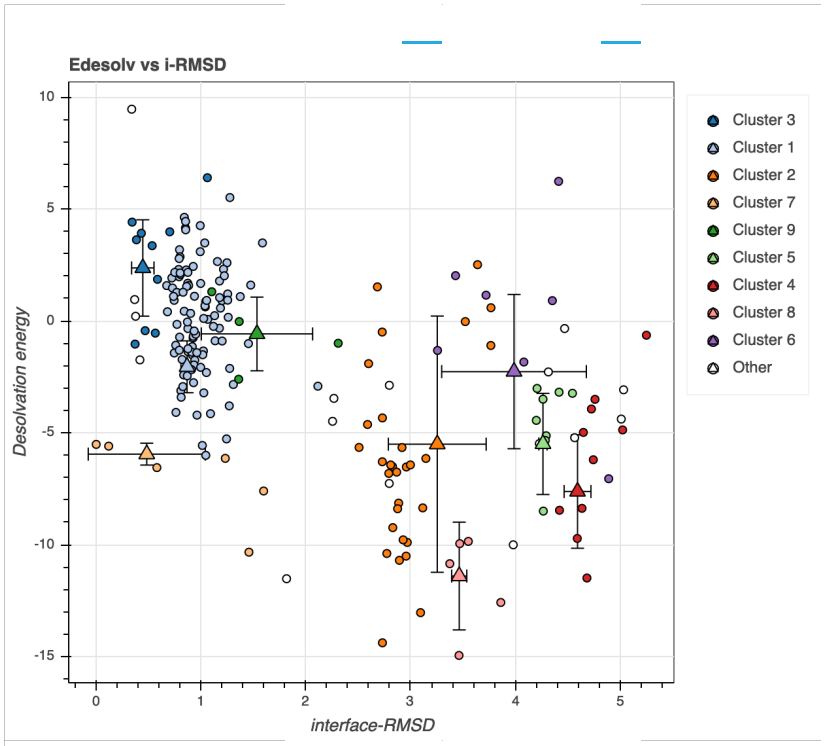
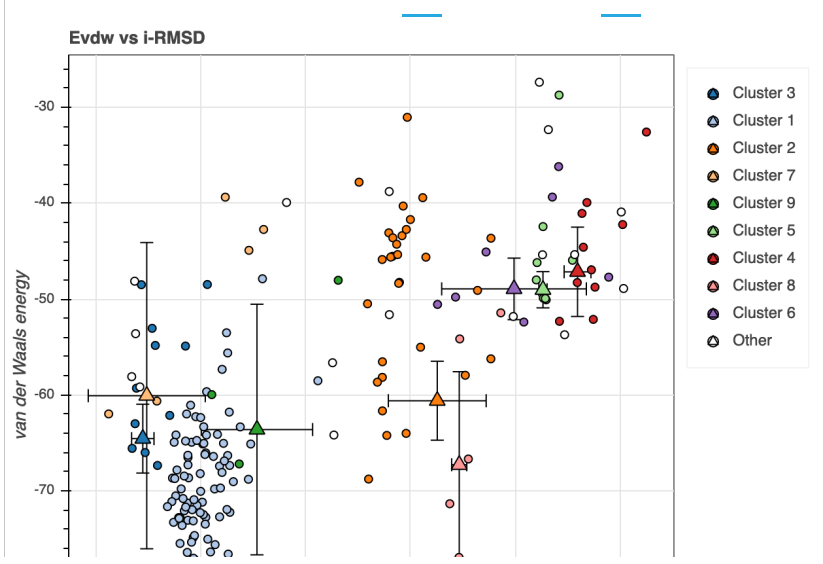
Model Analysis (Download all plots)

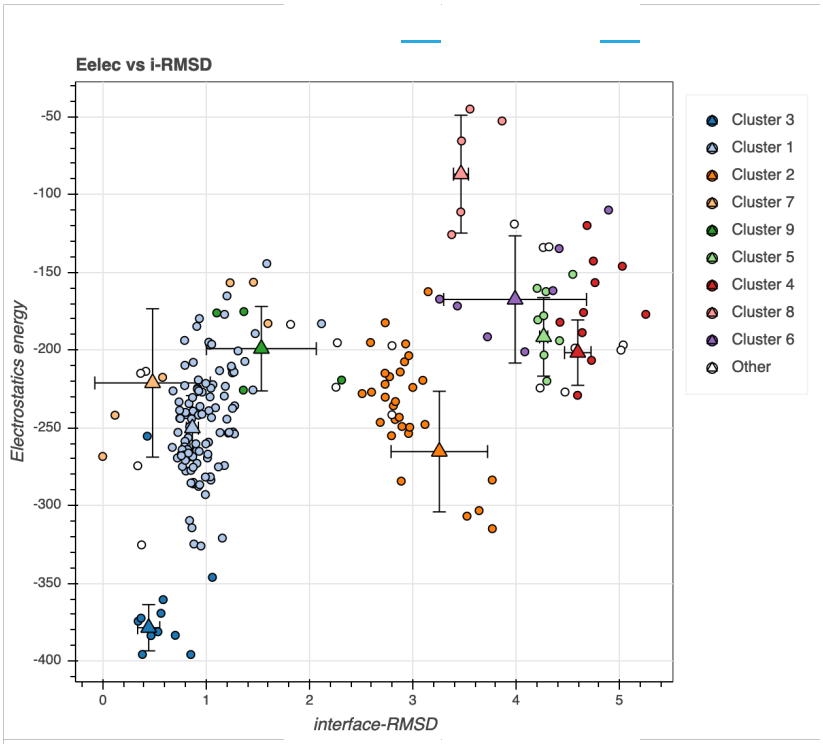
All | None | Cluster 3 | Cluster 1 | Cluster 2 | Cluster 7 | Cluster 9 | Cluster 5 | Cluster 4 | Cluster 8 | Cluster 6 | Ot

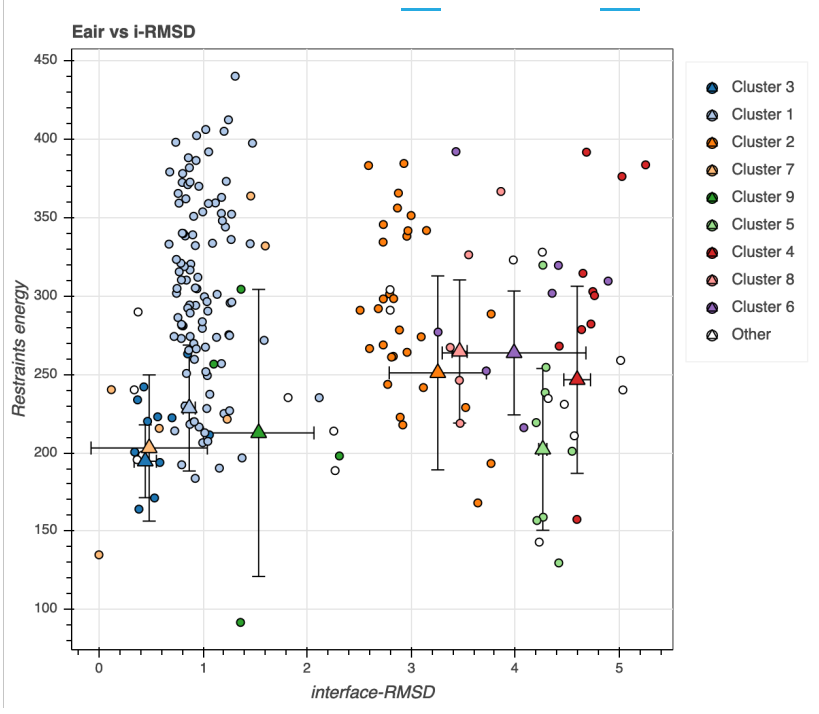





Edesolv vs i-RMSD
Desolvation energy
interface-RMSD
10
5
0
-5
-10
-15
0
1
2
3
4
5
Cluster 3
Cluster 1
Cluster 2
Cluster 7
Cluster 9
Cluster 5
Cluster 4
Cluster 8
Cluster 6
Other


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





Cluster Analysis

All	None	Cluster 3	Cluster 1	Cluster 2	Cluster 7	Cluster 9	Cluster 5	Cluster 4	Cluster 8	Cluster 6	Ot