HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_TCR-csp-35"

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 **179** structures in **8** cluster(s), which represents **89 %** 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	-90.2 +/- 3.4
Cluster size	57
RMSD from the overall lowest-energy structure	18.8 +/- 1.1
Van der Waals energy	-72.4 +/- 4.2
Electrostatic energy	-143.7 +/- 33.8
Desolvation energy	-14.7 +/- 2.2
Restraints violation energy	256.3 +/- 72.3
Buried Surface Area	1903.4 +/- 28.5
Z-Score	-1.1

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Nr 3 best structure Download file
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Cluster 3

HADDOCK score	-88.7 +/- 3.2
Cluster size	31
RMSD from the overall lowest-energy structure	19.7 +/- 0.4
Van der Waals energy	-79.7 +/- 6.5
Electrostatic energy	-145.1 +/- 10.1
Desolvation energy	-7.0 +/- 0.8
Restraints violation energy	270.0 +/- 57.3
Buried Surface Area	1969.2 +/- 31.9
Z-Score	-0.9

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Cluster 6

HADDOCK score	-88.1 +/- 6.1
Cluster size	6
RMSD from the overall lowest-energy structure	0.5 +/- 0.4
Van der Waals energy	-71.2 +/- 6.4
Electrostatic energy	-190.1 +/- 27.9
Desolvation energy	-4.7 +/- 0.5
Restraints violation energy	257.1 +/- 38.3
Buried Surface Area	2111.0 +/- 37.5

Z-Score	-0.9

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Cluster 2

HADDOCK score	-87.7 +/- 4.4
Cluster size	48
RMSD from the overall lowest-energy structure	12.2 +/- 0.3
Van der Waals energy	-74.0 +/- 4.0
Electrostatic energy	-141.7 +/- 5.0
Desolvation energy	-9.4 +/- 5.2
Restraints violation energy	239.8 +/- 37.7
Buried Surface Area	1827.1 +/- 123.1
Z-Score	-0.9

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Cluster 5

HADDOCK score	-74.8 +/- 14.5
Cluster size	8
RMSD from the overall lowest-energy structure	14.7 +/- 0.3
Van der Waals energy	-65.8 +/- 5.5
Electrostatic energy	-143.2 +/- 34.7
Desolvation energy	-18.0 +/- 2.5
Restraints violation energy	377.1 +/- 63.7
Buried Surface Area	1745.6 +/- 123.4
Z-Score	0.2

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Cluster 8

HADDOCK score	-65.9 +/- 10.2

Cluster size	4
RMSD from the overall lowest-energy structure	6.7 +/- 0.4
Van der Waals energy	-65.6 +/- 2.5
Electrostatic energy	-101.3 +/- 18.7
Desolvation energy	-9.4 +/- 1.4
Restraints violation energy	293.9 +/- 59.9
Buried Surface Area	1803.6 +/- 80.4
Z-Score	0.9

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Cluster 4

HADDOCK score	-64.4 +/- 1.8
Cluster size	20
RMSD from the overall lowest-energy structure	13.3 +/- 0.0
Van der Waals energy	-44.2 +/- 3.9
Electrostatic energy	-218.0 +/- 4.4
Desolvation energy	-9.1 +/- 1.8
Restraints violation energy	324.7 +/- 31.8
Buried Surface Area	1642.2 +/- 38.3
Z-Score	1.0

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Nr 4 best structure Download file

Cluster 7

HADDOCK score	-57.0 +/- 7.1
Cluster size	5
RMSD from the overall lowest-energy structure	5.2 +/- 0.3
Van der Waals energy	-54.1 +/- 3.4
Electrostatic energy	-98.2 +/- 16.4
Desolvation energy	-8.3 +/- 2.8
Restraints violation energy	250.6 +/- 26.3
Buried Surface Area	1649.6 +/- 120.6
Z-Score	1.6

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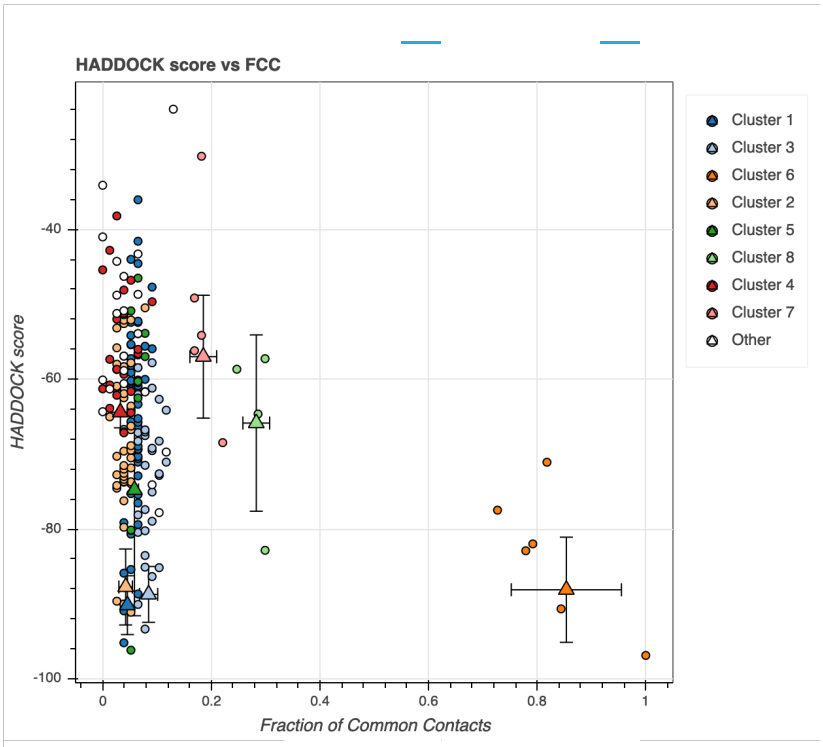
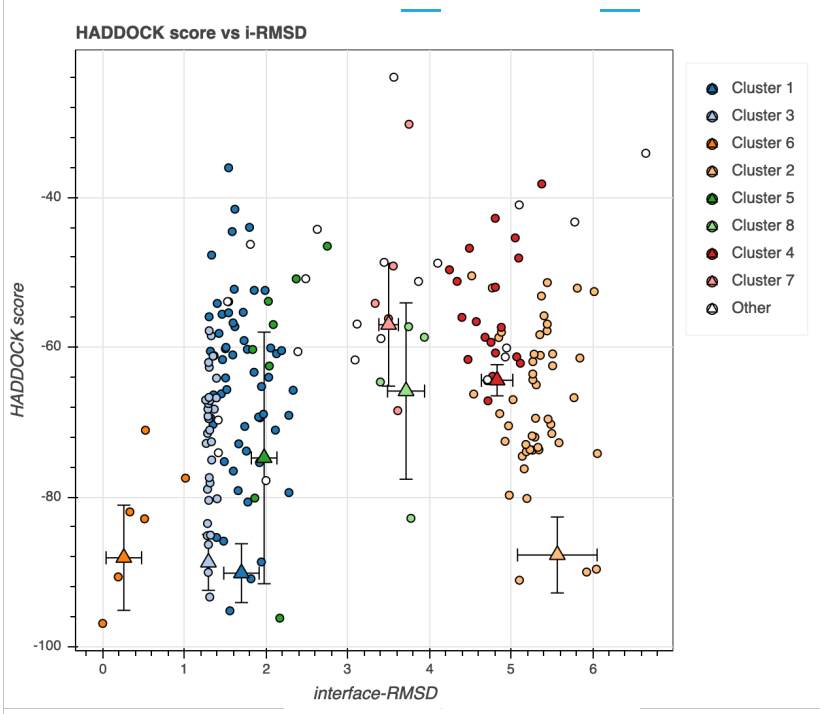
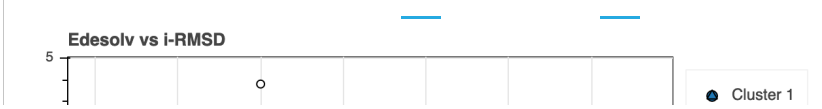
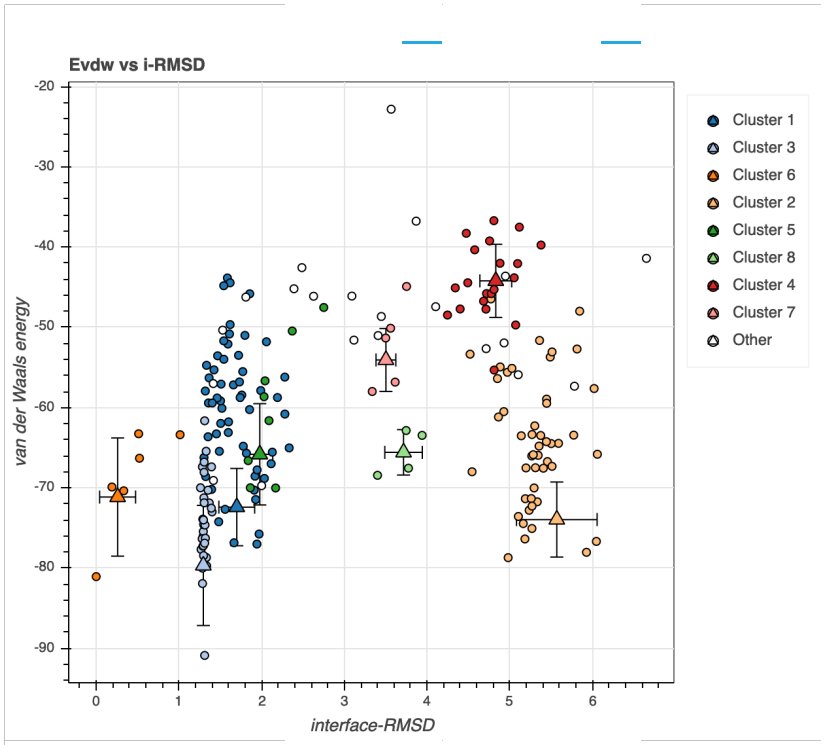
Model Analysis (Download all plots)

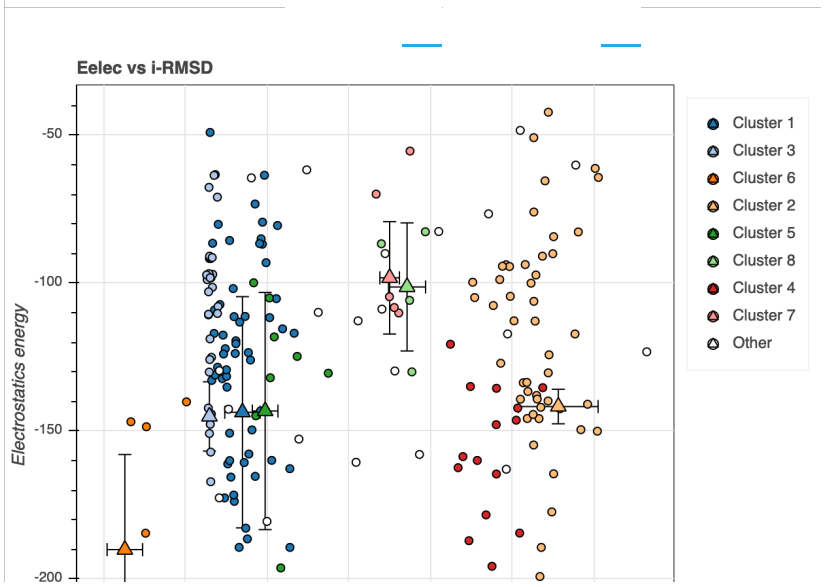
All | None | Cluster 1 | Cluster 3 | Cluster 6 | Cluster 2 | Cluster 5 | Cluster 8 | Cluster 4 | Cluster 7 | Oth

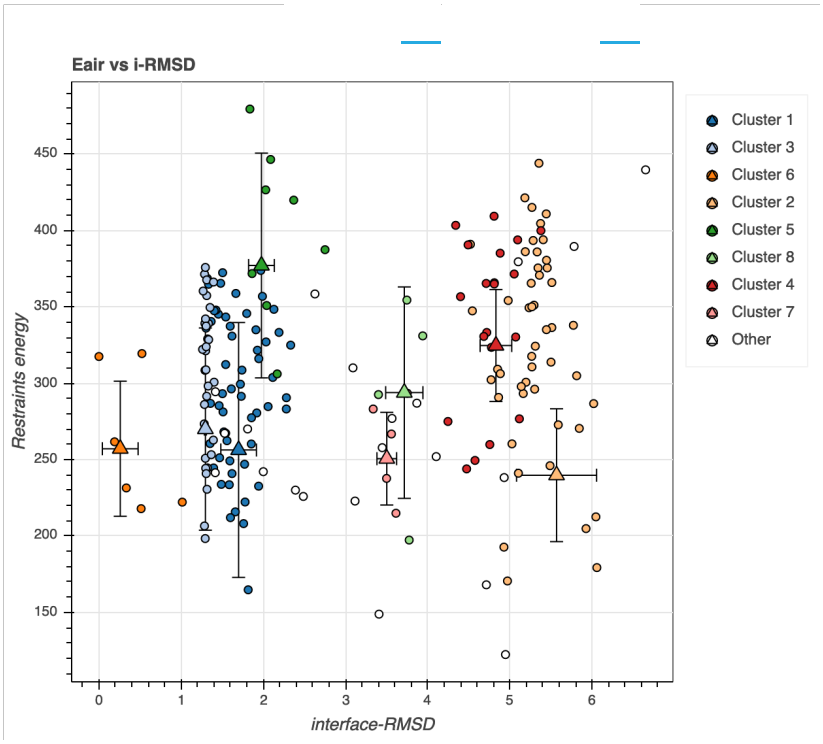






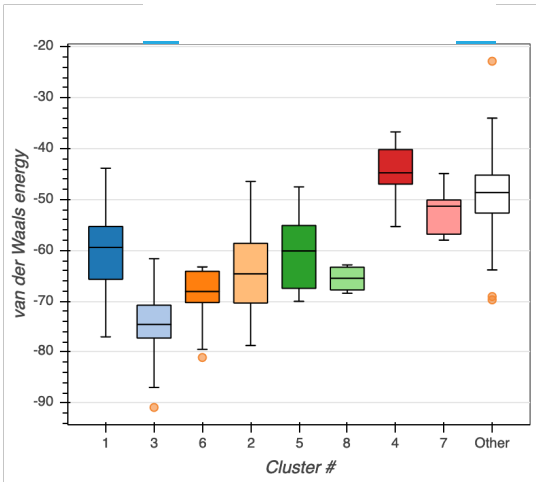

Evdw vs i-RMSD
van der Waals energy
interface-RMSD
-20
-30
-40
-50
-60
-70
-80
-90
0
1
2
3
4
5
6
Cluster 1
Cluster 3
Cluster 6
Cluster 2
Cluster 5
Cluster 8
Cluster 4
Cluster 7
Other

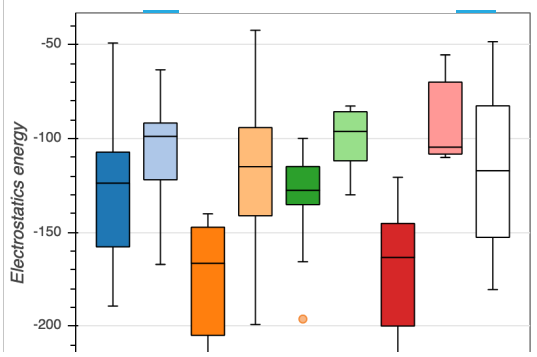

Eelec vs i-RMSD
Electrostatics energy
-50
-100
-150
-200
Cluster 1
Cluster 3
Cluster 6
Cluster 2
Cluster 5
Cluster 8
Cluster 4
Cluster 7
Other

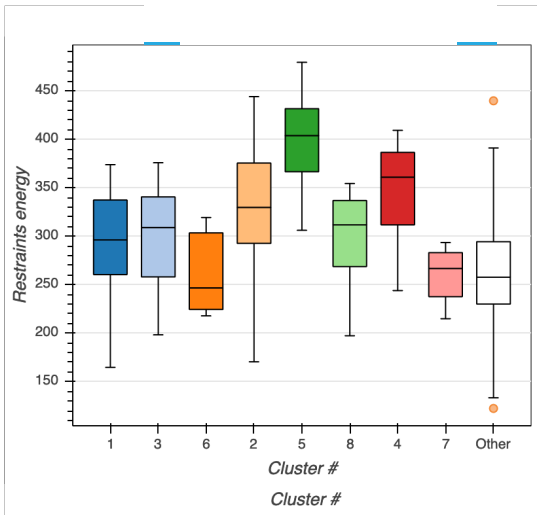


Cluster Analysis

All	None	Cluster 1	Cluster 3	Cluster 6	Cluster 2	Cluster 5	Cluster 8	Cluster 4	Cluster 7	Oth






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