HADDOCK 2.4

@Bonvinlab

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HADDOCK server status for job "cford_TCR-csp-12"

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 **176** structures in **8** cluster(s), which represents **88 %** 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	-102.5 +/- 2.1
Cluster size	121
RMSD from the overall lowest-energy structure	3.3 +/- 0.2
Van der Waals energy	-85.1 +/- 2.2
Electrostatic energy	-236.7 +/- 10.8
Desolvation energy	-5.4 +/- 1.6
Restraints violation energy	353.8 +/- 32.3

Buried Surface Area	2100.9 +/- 34.6
Z-Score	-2.0

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Cluster 2

HADDOCK score	-85.7 +/- 7.0
Cluster size	13
RMSD from the overall lowest-energy structure	18.5 +/- 0.5
Van der Waals energy	-62.4 +/- 4.6
Electrostatic energy	-219.2 +/- 50.5
Desolvation energy	-1.8 +/- 3.8
Restraints violation energy	222.7 +/- 44.2
Buried Surface Area	1811.0 +/- 83.7
Z-Score	-0.9

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Cluster 3

HADDOCK score	-79.9 +/- 5.9
Cluster size	12
RMSD from the overall lowest-energy structure	7.3 +/- 0.2
Van der Waals energy	-67.6 +/- 2.7
Electrostatic energy	-155.8 +/- 19.9
Desolvation energy	-2.4 +/- 3.0
Restraints violation energy	211.9 +/- 34.4
Buried Surface Area	1849.0 +/- 134.7
Z-Score	-0.5

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Cluster 6

HADDOCK score	-68.6 +/- 8.7
Cluster size	5
RMSD from the overall lowest-energy structure	9.5 +/- 0.6
Van der Waals energy	-63.6 +/- 5.9
Electrostatic energy	-172.6 +/- 18.4
Desolvation energy	-0.9 +/- 2.0
Restraints violation energy	303.8 +/- 67.7
Buried Surface Area	1965.9 +/- 69.3
Z-Score	0.2

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Cluster 4

HADDOCK score	-64.3 +/- 6.5
Cluster size	9
RMSD from the overall lowest-energy structure	18.3 +/- 0.5
Van der Waals energy	-58.5 +/- 2.9
Electrostatic energy	-88.5 +/- 7.2
Desolvation energy	-14.9 +/- 2.3
Restraints violation energy	267.4 +/- 32.9
Buried Surface Area	1680.9 +/- 88.1
Z-Score	0.5

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Cluster 7

HADDOCK score	-63.6 +/- 1.9
Cluster size	5
RMSD from the overall lowest-energy structure	13.8 +/- 0.5
Van der Waals energy	-52.8 +/- 1.8
Electrostatic energy	-124.3 +/- 25.2
Desolvation energy	-10.0 +/- 2.5
Restraints violation energy	240.5 +/- 39.4

Buried Surface Area	1559.5 +/- 57.0
Z-Score	0.6

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Cluster 8

HADDOCK score	-59.4 +/- 9.5
Cluster size	4
RMSD from the overall lowest-energy structure	4.8 +/- 0.9
Van der Waals energy	-57.7 +/- 8.1
Electrostatic energy	-91.5 +/- 15.9
Desolvation energy	-15.0 +/- 1.0
Restraints violation energy	317.0 +/- 14.1
Buried Surface Area	1673.8 +/- 58.2
Z-Score	0.8

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Cluster 5

HADDOCK score	-52.3 +/- 3.8
Cluster size	7
RMSD from the overall lowest-energy structure	6.9 +/- 0.2
Van der Waals energy	-49.3 +/- 4.5
Electrostatic energy	-146.8 +/- 42.4
Desolvation energy	-6.2 +/- 2.6
Restraints violation energy	325.5 +/- 20.7
Buried Surface Area	1612.1 +/- 14.3
Z-Score	1.3

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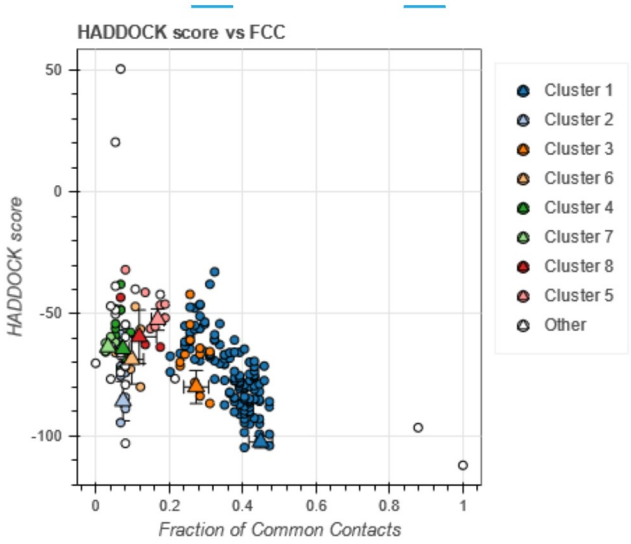
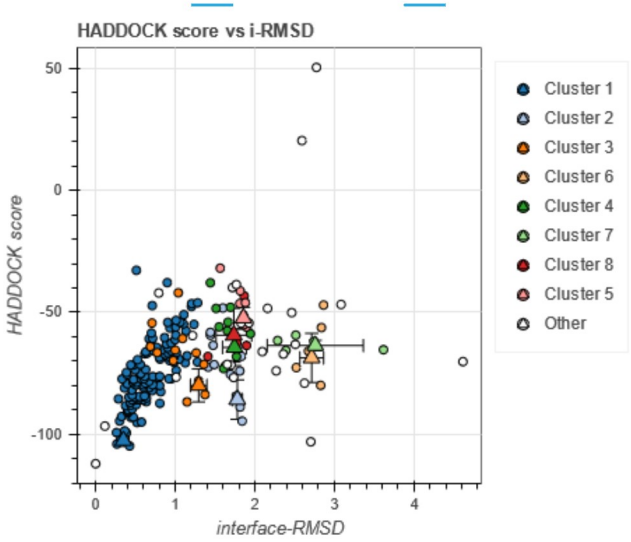
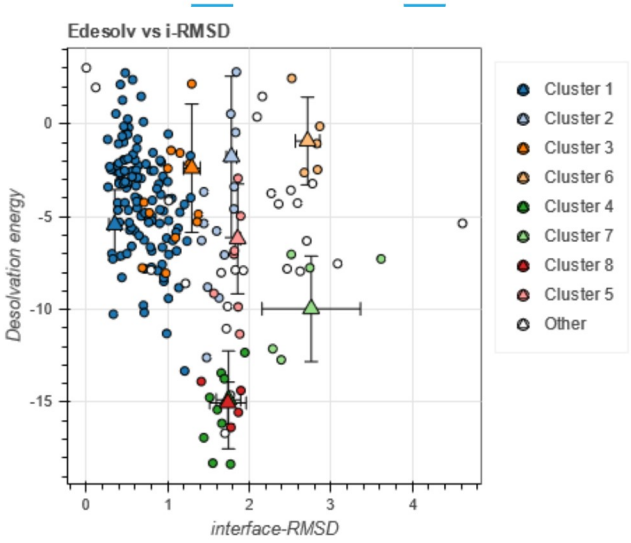
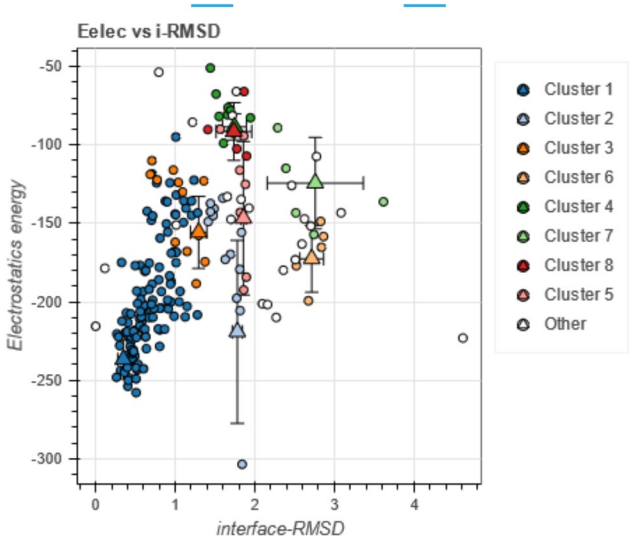
Model Analysis (Download all plots)

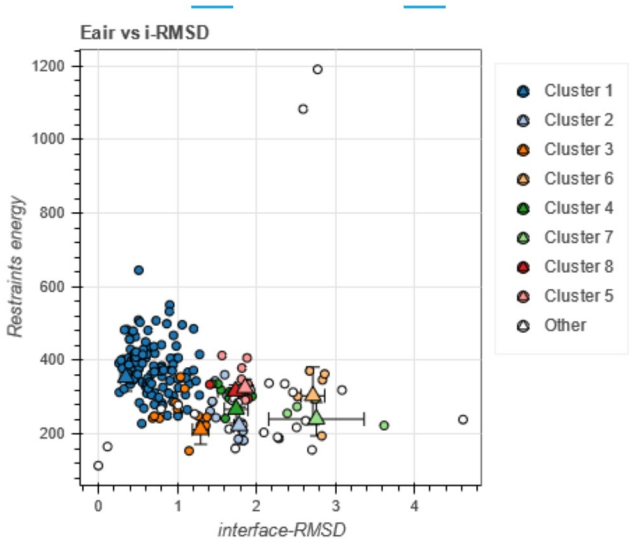
All | None | Cluster 1 | Cluster 2 | Cluster 3 | Cluster 6 | Cluster 4 | Cluster 7 | Cluster 8 | Cluster 5 | Other











Cluster Analysis

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