HADDOCK 2.4

@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for job "cford_HLA-csp-22"

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 **164** structures in **9** cluster(s), which represents **82 %** 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 5

HADDOCK score	-74.6 +/- 2.8
Cluster size	12
RMSD from the overall lowest-energy structure	0.3 +/- 0.2
Van der Waals energy	-26.7 +/- 5.4
Electrostatic energy	-262.8 +/- 28.4
Desolvation energy	2.0 +/- 1.7

Restraints violation energy	26.3 +/- 23.1
Buried Surface Area	1192.6 +/- 58.0
Z-Score	-1.3

Nr 1 best structure		Download file
Nr 2 best structure		Download file
Nr 3 best structure		Download file
Nr 4 best structure		Download file

Cluster 1

HADDOCK score	-68.7 +/- 2.6
Cluster size	48
RMSD from the overall lowest-energy structure	3.0 +/- 0.1
Van der Waals energy	-34.5 +/- 5.3
Electrostatic energy	-159.0 +/- 18.2
Desolvation energy	-4.4 +/- 2.0
Restraints violation energy	20.0 +/- 17.2
Buried Surface Area	1177.4 +/- 57.6
Z-Score	-0.6

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Cluster 7

HADDOCK score	-68.1 +/- 3.9
Cluster size	7
RMSD from the overall lowest-energy structure	3.0 +/- 0.0
Van der Waals energy	-33.3 +/- 5.3
Electrostatic energy	-165.3 +/- 44.3
Desolvation energy	-3.7 +/- 2.8
Restraints violation energy	19.6 +/- 13.5
Buried Surface Area	1458.5 +/- 40.2
Z-Score	-0.5

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Cluster 6

HADDOCK score	-67.9 +/- 4.1
Cluster size	11
RMSD from the overall lowest-energy structure	2.6 +/- 0.0
Van der Waals energy	-36.9 +/- 2.2
Electrostatic energy	-124.7 +/- 13.3
Desolvation energy	-7.5 +/- 1.5
Restraints violation energy	14.9 +/- 8.5
Buried Surface Area	1320.7 +/- 57.1
Z-Score	-0.5

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Cluster 3

HADDOCK score	-65.8 +/- 2.1
Cluster size	28
RMSD from the overall lowest-energy structure	0.8 +/- 0.1
Van der Waals energy	-34.3 +/- 2.0
Electrostatic energy	-124.3 +/- 13.5
Desolvation energy	-8.3 +/- 1.2
Restraints violation energy	16.6 +/- 14.4
Buried Surface Area	1241.1 +/- 24.6
Z-Score	-0.2

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Cluster 2

HADDOCK score	-64.3 +/- 0.9
Cluster size	35
RMSD from the overall lowest-energy structure	2.9 +/- 0.0
Van der Waals energy	-23.1 +/- 3.4

Electrostatic energy	-201.6 +/- 23.3
Desolvation energy	-2.1 +/- 1.3
Restraints violation energy	11.4 +/- 1.1
Buried Surface Area	1303.8 +/- 76.4
Z-Score	-0.0

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Cluster 4

HADDOCK score	-61.8 +/- 3.4
Cluster size	14
RMSD from the overall lowest-energy structure	2.5 +/- 0.2
Van der Waals energy	-41.0 +/- 3.5
Electrostatic energy	-78.8 +/- 31.2
Desolvation energy	-5.3 +/- 3.2
Restraints violation energy	1.8 +/- 0.9
Buried Surface Area	1153.9 +/- 54.1
Z-Score	0.3

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Cluster 8

HADDOCK score	-59.9 +/- 7.2
Cluster size	5
RMSD from the overall lowest-energy structure	3.4 +/- 0.2
Van der Waals energy	-25.2 +/- 10.2
Electrostatic energy	-178.9 +/- 38.1
Desolvation energy	-0.8 +/- 4.8
Restraints violation energy	18.8 +/- 14.0
Buried Surface Area	1219.6 +/- 102.7
Z-Score	0.5

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Cluster 9

HADDOCK score	-44.7 +/- 5.8
Cluster size	4
RMSD from the overall lowest-energy structure	2.9 +/- 0.1
Van der Waals energy	-23.4 +/- 3.4
Electrostatic energy	-123.2 +/- 43.1
Desolvation energy	0.9 +/- 2.9
Restraints violation energy	24.5 +/- 17.6
Buried Surface Area	1110.8 +/- 108.7
Z-Score	2.4

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Model Analysis (Download all plots)

Cluster Analysis