

HADDOCK2.2

WeNMR/West-Life GRID-enabled web portal

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HADDOCK server status for docking run /5763854415/GSTA1MAPK8apo

Status: FINISHED

Your HADDOCK run has successfully completed. The complete run can be downloaded as a gzipped tar file [here](#) (Note that there might be a delay in the generation of this archive - in case of errors try again). The file containing your docking parameters is [here](#).

Please cite the following papers in your work:

- G.C.P van Zundert, J.P.G.L.M. Rodrigues, M. Trellet, C. Schmitz, P.L. Kastiris, 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).
- Wassenaar et al., *WeNMR: Structural Biology on the Grid*. *J. Grid. Comp.*, **10**, 743-767 (2012).

And for the use of the WeNMR Grid resources please add the following acknowledgement:

"The FP7 WeNMR (project# 261572) and H2020 West-Life (project# 675858) European e-Infrastructure projects are acknowledged for the use of their web portals, which make use of the EGI infrastructure and the DIRAC4EGI service with the dedicated support of CESNET-MetaCloud, INFN-PADOVA, NCG-INGRID-PT, RAL-LCG2, TW-NCHC, IFCA-LCG2, SURFsara and NIKHEF, and the additional support of the national GRID Initiatives of Belgium, France, Italy, Germany, the Netherlands, Poland, Portugal, Spain, UK, South Africa, Malaysia, Taiwan and the US Open Science Grid."

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Summary

HADDOCK clustered **171** structures in **12** cluster(s), which represents **85.5 %** 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.

C L U S T E R 2

HADDOCK score	-83.7 +/- 6.2
Cluster size	15
RMSD from the overall lowest-energy structure	16.9 +/- 0.2
Van der Waals energy	-98.2 +/- 11.0
Electrostatic energy	-289.4 +/- 36.2
Desolvation energy	-4.7 +/- 1.1
Restraints violation energy	770.8 +/- 244.83
Buried Surface Area	3402.6 +/- 343.3
Z-Score	-1.5

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C L U S T E R 7

HADDOCK score	-81.1 +/- 8.5
Cluster size	6
RMSD from the overall lowest-energy structure	6.9 +/- 0.2
Van der Waals energy	-104.5 +/- 4.3
Electrostatic energy	-266.8 +/- 22.1
Desolvation energy	11.4 +/- 4.1
Restraints violation energy	654.1 +/- 72.16
Buried Surface Area	3303.1 +/- 111.0
Z-Score	-1.3

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C L U S T E R 3

HADDOCK score	-71.5 +/- 14.6
Cluster size	10
RMSD from the overall lowest-energy structure	15.6 +/- 0.1
Van der Waals energy	-105.2 +/- 7.5
Electrostatic energy	-275.6 +/- 49.1
Desolvation energy	0.2 +/- 5.6
Restraints violation energy	886.0 +/- 49.61
Buried Surface Area	3286.0 +/- 176.0
Z-Score	-0.8

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C L U S T E R 9

HADDOCK score	-70.2 +/- 20.6
Cluster size	4
RMSD from the overall lowest-energy structure	1.6 +/- 1.0
Van der Waals energy	-98.7 +/- 11.9
Electrostatic energy	-267.3 +/- 101.3
Desolvation energy	-9.4 +/- 16.5
Restraints violation energy	914.4 +/- 77.85
Buried Surface Area	3336.1 +/- 106.8
Z-Score	-0.7

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C L U S T E R 1

HADDOCK score	-61.3 +/- 0.9
Cluster size	97
RMSD from the overall lowest-energy structure	15.9 +/- 0.4
Van der Waals energy	-90.0 +/- 2.5
Electrostatic energy	-290.3 +/- 62.4

Desolvation energy	3.9 +/- 5.4
Restraints violation energy	828.6 +/- 95.12
Buried Surface Area	2686.3 +/- 85.6
Z-Score	-0.3

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C L U S T E R 4

HADDOCK score	-50.6 +/- 27.3
Cluster size	7
RMSD from the overall lowest-energy structure	13.5 +/- 0.9
Van der Waals energy	-89.0 +/- 7.4
Electrostatic energy	-301.7 +/- 83.7
Desolvation energy	13.5 +/- 10.1
Restraints violation energy	852.9 +/- 23.23
Buried Surface Area	3073.7 +/- 55.0
Z-Score	0.3

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C L U S T E R 1 1

HADDOCK score	-40.0 +/- 5.3
Cluster size	4
RMSD from the overall lowest-energy structure	15.9 +/- 0.2
Van der Waals energy	-90.6 +/- 7.4
Electrostatic energy	-265.1 +/- 15.9
Desolvation energy	19.2 +/- 2.6
Restraints violation energy	844.3 +/- 62.59
Buried Surface Area	3117.6 +/- 305.5
Z-Score	0.9

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C L U S T E R 8

HADDOCK score	-39.3 +/- 8.6
Cluster size	6
RMSD from the overall lowest-energy structure	15.5 +/- 0.1
Van der Waals energy	-77.6 +/- 7.5
Electrostatic energy	-221.3 +/- 6.8
Desolvation energy	-1.9 +/- 8.8
Restraints violation energy	844.5 +/- 95.54
Buried Surface Area	2487.5 +/- 198.3
Z-Score	0.9

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C L U S T E R 5

HADDOCK score	-36.3 +/- 3.4
Cluster size	7
RMSD from the overall lowest-energy structure	16.0 +/- 0.1
Van der Waals energy	-96.0 +/- 5.5
Electrostatic energy	-202.0 +/- 49.4
Desolvation energy	4.7 +/- 3.5
Restraints violation energy	954.5 +/- 45.48
Buried Surface Area	3080.5 +/- 118.1
Z-Score	1.1

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C L U S T E R 1 0

HADDOCK score	-30.2 +/- 17.1
Cluster size	4
RMSD from the overall lowest-energy structure	13.3 +/- 0.5
Van der Waals energy	-91.3 +/- 17.1
Electrostatic energy	-240.0 +/- 42.3
Desolvation energy	18.8 +/- 13.1
Restraints violation energy	903.4 +/- 51.51
Buried Surface Area	3210.2 +/- 393.8
Z-Score	1.4

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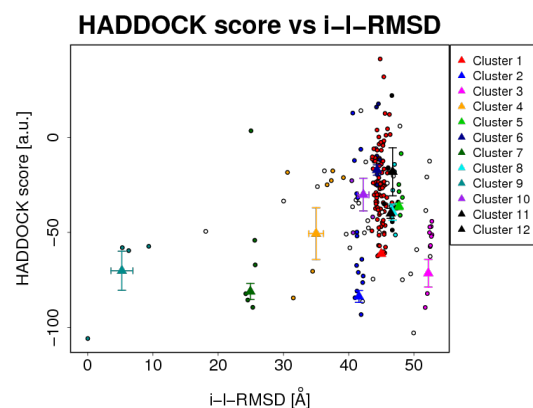
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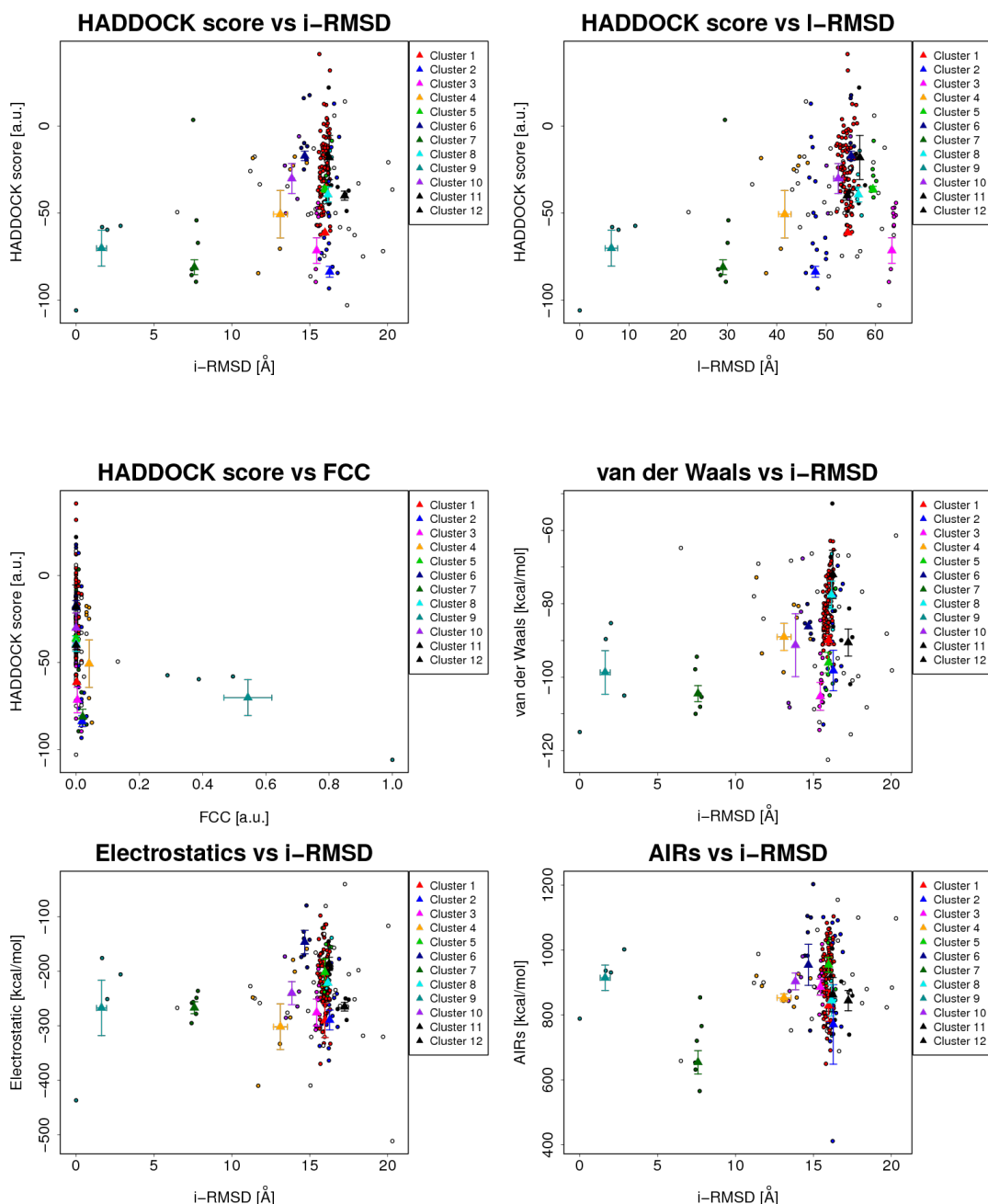
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R E S U L T S A N A L Y S I S

The results and graphics presented below are based on water-refined models generated by HADDOCK. The clusters (indicated in color in the graphs) are calculated based on the interface-ligand RMSDs calculated by HADDOCK, with the interface defined automatically based on all observed contacts. The various structural analysis ([FCC](#), [i-RMSD](#) and [I-RMSD](#)) are made with respect to the best HADDOCK model (the one with the lowest HADDOCK score).





S U P P L E M E N T A R Y I N F O R M

i-RMSD -> interface-RMSD calculated on the backbone (CA,C,N,O,P) atoms of all residues involved in intermolecular contact using a 10Å cutoff

I-RMSD -> ligand-RMSD calculated on the backbone atoms (CA,C,N,O,P) of all (N>1) molecules after fitting on the backbone atoms of the first (N=1) molecule

FCC -> Fraction of common contacts. The intermolecular contacts are defined based on the best HADDOCK model using a 5Å cutoff (see [Rodrigues et al, Proteins 2012](#))

a.u. -> Arbitrary Units

The cluster averages and standard deviations are indicated by colored dots with associated error bars. The average values are calculated on the best 4 structures of each clusters (based on the HADDOCK score).

Note that HADDOCK results are deleted after one week.

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