

HADDOCK2.2

WeNMR/West-Life GRID-enabled web portal

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HADDOCK server status for docking run /5763854415/GSTM1ASK1APOFINAL

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:

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Summary

HADDOCK clustered **157** structures in **15** cluster(s), which represents **78.5 %** 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 1

HADDOCK score	-68.3 +/- 11.0
Cluster size	32
RMSD from the overall lowest-energy structure	7.3 +/- 0.2
Van der Waals energy	-101.9 +/- 4.9
Electrostatic energy	-542.2 +/- 20.7
Desolvation energy	13.7 +/- 8.3
Restraints violation energy	1283.1 +/- 85.59
Buried Surface Area	3565.7 +/- 286.0
Z-Score	-1.7

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C L U S T E R 4

HADDOCK score	-55.4 +/- 7.1
Cluster size	14
RMSD from the overall lowest-energy structure	3.0 +/- 1.4
Van der Waals energy	-95.9 +/- 6.1
Electrostatic energy	-370.6 +/- 63.0
Desolvation energy	-13.6 +/- 7.3
Restraints violation energy	1282.7 +/- 100.76
Buried Surface Area	3482.8 +/- 193.6
Z-Score	-1.1

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C L U S T E R 5

HADDOCK score	-50.1 +/- 7.8
Cluster size	14
RMSD from the overall lowest-energy structure	19.1 +/- 0.1
Van der Waals energy	-97.9 +/- 8.7
Electrostatic energy	-592.5 +/- 34.6
Desolvation energy	17.5 +/- 6.7
Restraints violation energy	1487.7 +/- 112.58
Buried Surface Area	3677.1 +/- 140.1
Z-Score	-0.8

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C L U S T E R 1 0

HADDOCK score	-45.1 +/- 9.8
Cluster size	8
RMSD from the overall lowest-energy structure	13.0 +/- 0.1
Van der Waals energy	-111.0 +/- 6.2
Electrostatic energy	-456.6 +/- 91.3
Desolvation energy	7.6 +/- 6.2
Restraints violation energy	1497.0 +/- 89.27
Buried Surface Area	3527.6 +/- 197.3
Z-Score	-0.6

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C L U S T E R 3

HADDOCK score	-38.0 +/- 10.2
Cluster size	14
RMSD from the overall lowest-energy structure	10.9 +/- 0.2
Van der Waals energy	-109.7 +/- 12.9
Electrostatic energy	-382.7 +/- 78.7

Desolvation energy	7.7 +/- 7.5
Restraints violation energy	1405.5 +/- 62.41
Buried Surface Area	3265.5 +/- 237.6
Z-Score	-0.2

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C L U S T E R 8

HADDOCK score	-32.3 +/- 10.9
Cluster size	9
RMSD from the overall lowest-energy structure	17.9 +/- 0.1
Van der Waals energy	-96.6 +/- 9.2
Electrostatic energy	-445.4 +/- 35.7
Desolvation energy	12.2 +/- 4.6
Restraints violation energy	1411.6 +/- 86.15
Buried Surface Area	3130.4 +/- 117.9
Z-Score	0.1

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C L U S T E R 1 1

HADDOCK score	-14.4 +/- 20.9
Cluster size	5
RMSD from the overall lowest-energy structure	19.7 +/- 0.4
Van der Waals energy	-103.8 +/- 17.0
Electrostatic energy	-396.4 +/- 65.8
Desolvation energy	19.6 +/- 4.9
Restraints violation energy	1490.1 +/- 89.72
Buried Surface Area	3569.4 +/- 304.0
Z-Score	0.9

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C L U S T E R 7

HADDOCK score	-14.1 +/- 25.9
Cluster size	10
RMSD from the overall lowest-energy structure	20.3 +/- 0.1
Van der Waals energy	-78.0 +/- 11.2
Electrostatic energy	-562.2 +/- 92.3
Desolvation energy	23.5 +/- 6.8
Restraints violation energy	1527.6 +/- 88.23
Buried Surface Area	3384.8 +/- 317.1
Z-Score	1.0

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C L U S T E R 2

HADDOCK score	-14.1 +/- 6.7
Cluster size	15
RMSD from the overall lowest-energy structure	20.1 +/- 0.3
Van der Waals energy	-88.2 +/- 9.8
Electrostatic energy	-303.3 +/- 104.3
Desolvation energy	-12.5 +/- 12.1
Restraints violation energy	1472.6 +/- 136.72
Buried Surface Area	2955.7 +/- 101.0
Z-Score	1.0

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C L U S T E R 1 3

HADDOCK score	-3.7 +/- 17.7
Cluster size	4
RMSD from the overall lowest-energy structure	23.2 +/- 0.1
Van der Waals energy	-87.1 +/- 3.7
Electrostatic energy	-328.4 +/- 49.1
Desolvation energy	-0.6 +/- 14.1
Restraints violation energy	1496.0 +/- 138.51
Buried Surface Area	2582.3 +/- 77.7
Z-Score	1.5

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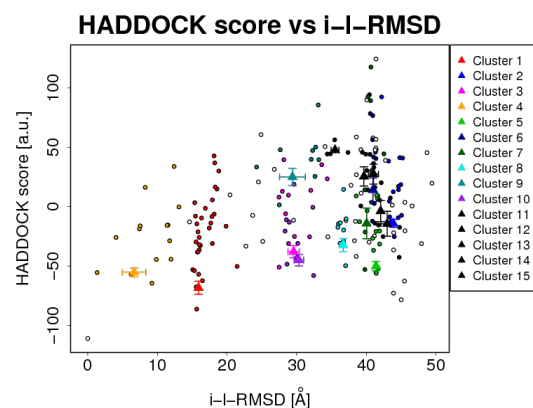
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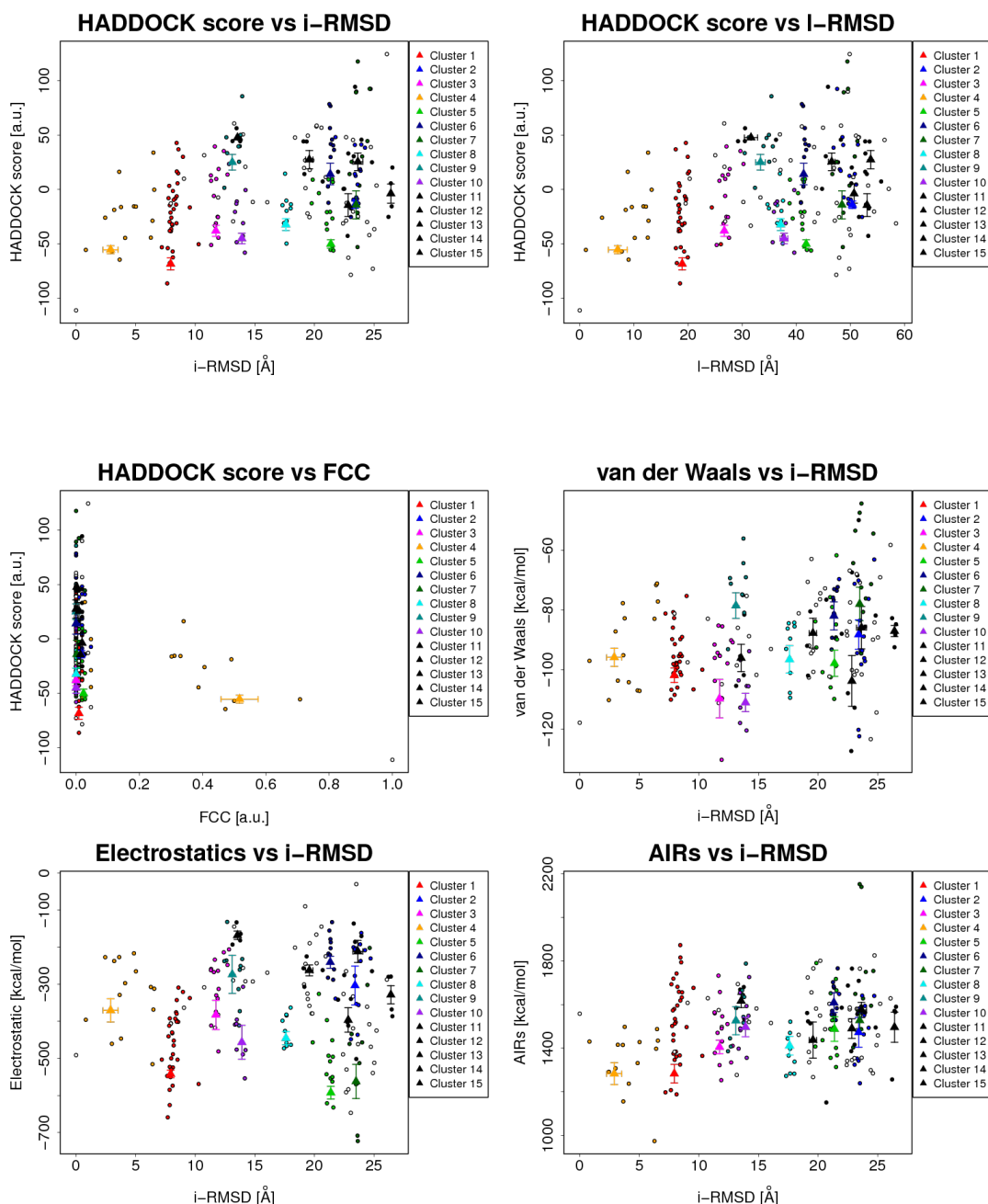
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R E S U L T S A N A L Y S I S

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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