

HADDOCK2.2

WeNMR/West-Life GRID-enabled web portal

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HADDOCK server status for docking run /5763854415/GSTTHETAASK1APO

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 **158** structures in **14** cluster(s), which represents **79.0 %** 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 3

HADDOCK score	-44.3 +/- 9.0
Cluster size	17
RMSD from the overall lowest-energy structure	0.7 +/- 0.4
Van der Waals energy	-103.0 +/- 1.5
Electrostatic energy	-456.7 +/- 32.2
Desolvation energy	-1.5 +/- 6.3
Restraints violation energy	1514.8 +/- 59.09
Buried Surface Area	3335.9 +/- 49.8
Z-Score	-1.5

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C L U S T E R 1 1

HADDOCK score	-38.0 +/- 8.8
Cluster size	5
RMSD from the overall lowest-energy structure	19.4 +/- 0.0
Van der Waals energy	-115.1 +/- 7.5
Electrostatic energy	-420.1 +/- 25.3
Desolvation energy	-14.2 +/- 4.5
Restraints violation energy	1753.3 +/- 124.28
Buried Surface Area	3582.2 +/- 84.4
Z-Score	-1.1

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C L U S T E R 4

HADDOCK score	-32.3 +/- 6.4
Cluster size	16
RMSD from the overall lowest-energy structure	7.9 +/- 2.3
Van der Waals energy	-91.0 +/- 8.9
Electrostatic energy	-507.5 +/- 76.5
Desolvation energy	-1.8 +/- 6.0
Restraints violation energy	1620.0 +/- 54.21
Buried Surface Area	3116.8 +/- 153.1
Z-Score	-0.7

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C L U S T E R 2

HADDOCK score	-29.4 +/- 7.7
Cluster size	24
RMSD from the overall lowest-energy structure	20.0 +/- 0.2
Van der Waals energy	-96.9 +/- 5.7
Electrostatic energy	-377.3 +/- 54.4
Desolvation energy	-14.7 +/- 3.8
Restraints violation energy	1575.7 +/- 131.18
Buried Surface Area	3153.2 +/- 77.0
Z-Score	-0.5

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C L U S T E R 8

HADDOCK score	-26.1 +/- 15.3
Cluster size	7
RMSD from the overall lowest-energy structure	17.8 +/- 0.1
Van der Waals energy	-91.9 +/- 7.5
Electrostatic energy	-426.8 +/- 57.2

Desolvation energy	1.3 +/- 5.8
Restraints violation energy	1499.0 +/- 120.52
Buried Surface Area	2927.5 +/- 72.0
Z-Score	-0.2

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C L U S T E R 6

HADDOCK score	-24.2 +/- 10.5
Cluster size	10
RMSD from the overall lowest-energy structure	17.3 +/- 0.5
Van der Waals energy	-94.9 +/- 7.5
Electrostatic energy	-462.2 +/- 60.1
Desolvation energy	14.4 +/- 6.8
Restraints violation energy	1487.6 +/- 105.29
Buried Surface Area	3233.8 +/- 216.6
Z-Score	-0.1

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C L U S T E R 5

HADDOCK score	-18.7 +/- 16.3
Cluster size	11
RMSD from the overall lowest-energy structure	19.1 +/- 0.5
Van der Waals energy	-99.7 +/- 5.2
Electrostatic energy	-375.3 +/- 33.8
Desolvation energy	1.6 +/- 12.4
Restraints violation energy	1543.8 +/- 165.31
Buried Surface Area	3304.6 +/- 162.7
Z-Score	0.3

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C L U S T E R 9

HADDOCK score	-16.6 +/- 14.4
Cluster size	6
RMSD from the overall lowest-energy structure	19.4 +/- 0.1
Van der Waals energy	-93.5 +/- 11.2
Electrostatic energy	-389.5 +/- 17.1
Desolvation energy	0.2 +/- 10.6
Restraints violation energy	1545.7 +/- 131.11
Buried Surface Area	3201.3 +/- 275.0
Z-Score	0.5

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C L U S T E R 1

HADDOCK score	-5.3 +/- 15.2
Cluster size	34
RMSD from the overall lowest-energy structure	20.9 +/- 0.1
Van der Waals energy	-105.4 +/- 11.7
Electrostatic energy	-272.2 +/- 92.9
Desolvation energy	2.5 +/- 9.0
Restraints violation energy	1520.2 +/- 117.46
Buried Surface Area	3032.0 +/- 287.6
Z-Score	1.3

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C L U S T E R 7

HADDOCK score	3.0 +/- 20.1
Cluster size	9
RMSD from the overall lowest-energy structure	20.0 +/- 0.3
Van der Waals energy	-80.5 +/- 4.0
Electrostatic energy	-325.7 +/- 75.9
Desolvation energy	-3.6 +/- 8.9
Restraints violation energy	1523.1 +/- 73.05
Buried Surface Area	2779.3 +/- 115.6
Z-Score	1.9

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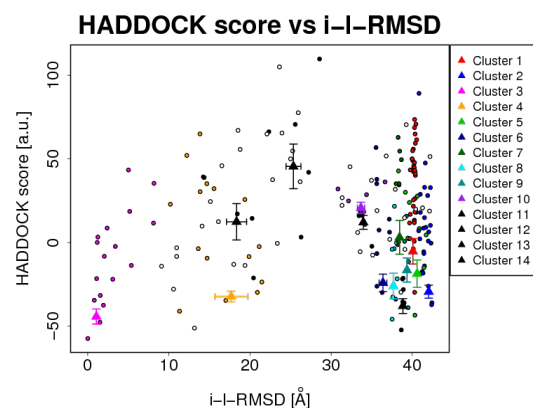
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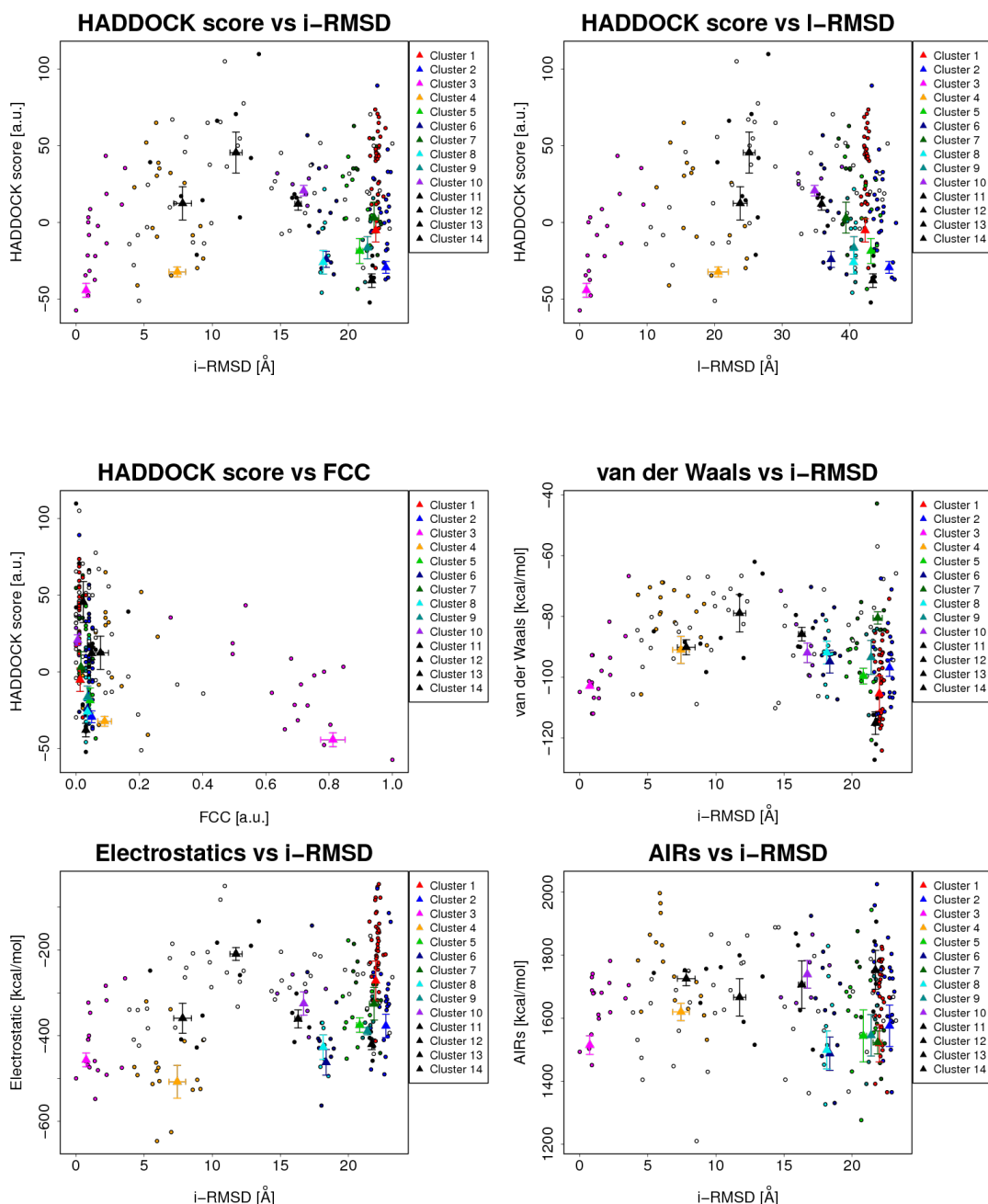
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R E S U L T S A N A L Y S I S

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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