

HADDOCK2.2

WeNMR/West-Life GRID-enabled web portal

WeNMR
homeWest-Life
home

West-Life services

HADDOCK2.2

HADDOCK
tutorialsHADDOCK Support
Center

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

HADDOCK server status for docking run /5763854415/GSTA1ASK1APOFINAL

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."

Questions / feedback ? ask.bioexcel.eu

Please also consider giving us some feedback by filling our [online survey](#).

Summary

HADDOCK clustered **149** structures in **11** cluster(s), which represents **74.5 %** 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 7

HADDOCK score	-86.5 +/- 9.1
Cluster size	8
RMSD from the overall lowest-energy structure	13.6 +/- 0.2
Van der Waals energy	-119.7 +/- 8.8
Electrostatic energy	-771.8 +/- 44.6
Desolvation energy	31.9 +/- 1.5
Restraints violation energy	1556.2 +/- 164.82
Buried Surface Area	3999.6 +/- 139.5
Z-Score	-1.8

Nr 1 best structure [Download structure](#)



Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 1

HADDOCK score	-74.8 +/- 23.1
Cluster size	40

RMSD from the overall lowest-energy structure	1.8 +/- 1.8
Van der Waals energy	-100.8 +/- 6.0
Electrostatic energy	-407.2 +/- 84.5
Desolvation energy	-7.3 +/- 8.1
Restraints violation energy	1147.6 +/- 107.23
Buried Surface Area	3305.0 +/- 285.5
Z-Score	-1.5

Nr 1 best structure [Download structure](#)



Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 3

HADDOCK score	-38.7 +/- 14.3
Cluster size	17
RMSD from the overall lowest-energy structure	5.6 +/- 1.5
Van der Waals energy	-98.5 +/- 10.1
Electrostatic energy	-318.9 +/- 55.7
Desolvation energy	-20.0 +/- 12.0
Restraints violation energy	1435.4 +/- 101.49
Buried Surface Area	3447.3 +/- 345.9
Z-Score	-0.6

Nr 1 best structure [Download structure](#)



Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 1 0

HADDOCK score	-25.2 +/- 10.2
Cluster size	4
RMSD from the overall lowest-energy structure	18.8 +/- 0.0
Van der Waals energy	-93.2 +/- 14.2
Electrostatic energy	-498.9 +/- 69.2
Desolvation energy	12.9 +/- 9.6
Restraints violation energy	1549.2 +/- 89.92
Buried Surface Area	3645.6 +/- 289.2
Z-Score	-0.3

Nr 1 best structure [Download structure](#)



Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 2

HADDOCK score	-19.3 +/- 8.5
Cluster size	29
RMSD from the overall lowest-energy structure	18.0 +/- 0.4
Van der Waals energy	-87.2 +/- 5.5
Electrostatic energy	-433.8 +/- 53.4
Desolvation energy	14.4 +/- 1.2
Restraints violation energy	1402.5 +/- 112.98
Buried Surface Area	3217.2 +/- 190.8
Z-Score	-0.1

Nr 1 best structure [Download structure](#) 


Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 6

HADDOCK score	2.6 +/- 16.5
Cluster size	9
RMSD from the overall lowest-energy structure	9.2 +/- 0.8
Van der Waals energy	-89.5 +/- 11.7
Electrostatic energy	-346.6 +/- 49.5
Desolvation energy	9.9 +/- 6.5
Restraints violation energy	1514.8 +/- 92.72
Buried Surface Area	2914.3 +/- 96.2
Z-Score	0.4

Nr 1 best structure [Download structure](#) 


Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 5

HADDOCK score	5.9 +/- 4.8
Cluster size	12
RMSD from the overall lowest-energy structure	17.6 +/- 0.3
Van der Waals energy	-102.3 +/- 13.3
Electrostatic energy	-301.6 +/- 41.2
Desolvation energy	19.8 +/- 10.9
Restraints violation energy	1487.1 +/- 110.86
Buried Surface Area	3185.8 +/- 152.8
Z-Score	0.5

Nr 1 best structure [Download structure](#) 


Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 8

HADDOCK score	25.8 +/- 20.1
Cluster size	6
RMSD from the overall lowest-energy structure	6.2 +/- 1.4
Van der Waals energy	-66.7 +/- 14.9
Electrostatic energy	-366.9 +/- 62.8
Desolvation energy	6.1 +/- 12.5
Restraints violation energy	1598.3 +/- 222.06
Buried Surface Area	2644.2 +/- 282.3
Z-Score	1.0

Nr 1 best structure [Download structure](#) 

Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 4

HADDOCK score	29.2 +/- 7.2
Cluster size	15
RMSD from the overall lowest-energy structure	18.8 +/- 0.2
Van der Waals energy	-84.0 +/- 6.8
Electrostatic energy	-231.1 +/- 27.1
Desolvation energy	-1.9 +/- 7.5
Restraints violation energy	1614.2 +/- 60.61
Buried Surface Area	2801.4 +/- 135.3
Z-Score	1.1

Nr 1 best structure [Download structure](#)



Nr 2 best structure [Download structure](#)

Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

C L U S T E R 9

HADDOCK score	39.7 +/- 13.9
Cluster size	5
RMSD from the overall lowest-energy structure	18.4 +/- 0.0
Van der Waals energy	-77.4 +/- 10.7
Electrostatic energy	-232.7 +/- 76.0
Desolvation energy	-8.9 +/- 9.2
Restraints violation energy	1725.9 +/- 60.38
Buried Surface Area	2224.7 +/- 190.0
Z-Score	1.3

Nr 1 best structure [Download structure](#)



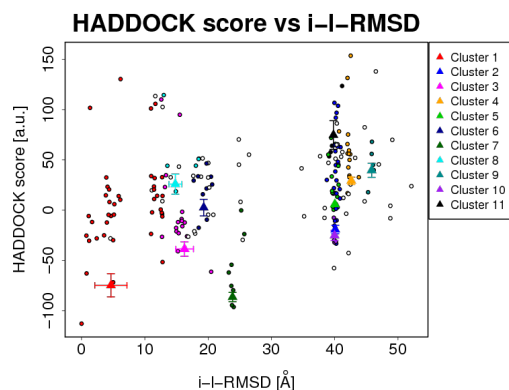
Nr 2 best structure [Download structure](#)

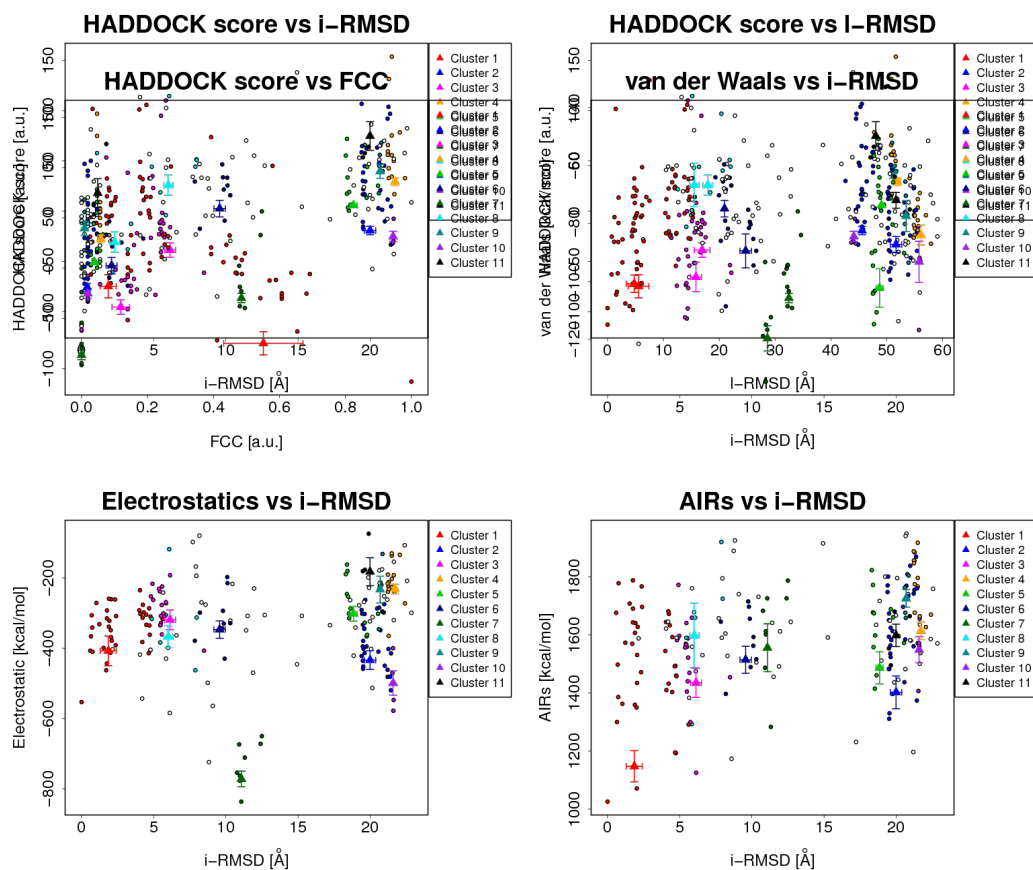
Nr 3 best structure [Download structure](#)

Nr 4 best structure [Download structure](#)

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.

[WeNMR home](#) [West-Life home](#) [West-Life services](#) [HADDOCK2.2](#) [HADDOCK tutorials](#) [HADDOCK Support Center](#)

2008-2017 © Computational Structural Biology group. All rights reserved. Original webdesign by Marc van Dijk
XHTML | CSS