Rapid determination of RMSDs corresponding to macromolecular rigid body motions

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SUPPLEMENTARY INFORMATION

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Table S1: Benchmark of protein complexes that were used during the clustering experiment.

Receptor[a]	Ligand[a]	Number of atoms in the ligand molecule[b]
1AYM::1	1AYM::2	1981
1AYM::2	1AYM::3	1847
1AYM::3	1AYM::1	2336
1B35::A	1B35::B	1412
1B35::B	1B35::C	2129
1B35::C	1B35::A	2029
1EPT::A	1EPT::B	768
1EPT::B	1EPT::C	863
1EPT::C	1EPT::A	388
1RM6::A	1RM6::B	2422
1RM6::B	1RM6::C	1178
1SR4::A	1SR4::B	2025
1SR4::B	1SR4::C	1203
1SR4::C	1SR4::A	1308
1W85::F	1W85::G	2569
1W85::G	1W85::H	2483
1W85::H	1W85::F	2473
2WJN::H	2WJN::L	2161
2WJN::L	2WJN::M	2451
2WJN::M	2WJN::H	1876
3VBH::A	3VBH::B	2300
3VBH::B	3VBH::C	1896
3VBH::C	3VBH::A	1863

[a] Protein code in the Protein Data Bank, followed by the protein chain identifier.

[b] After processing of the PDB file.

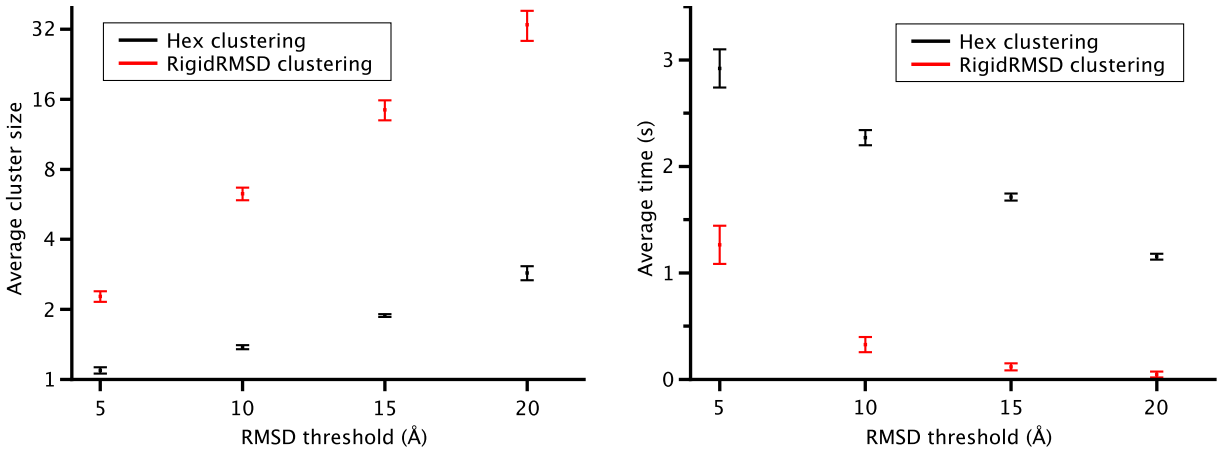

Figure S1. Comparison of clustering docking solutions for Hex and *RigidRMSD* with respect to the clustering RMSD threshold. Left: Average cluster size (on a logarithmic scale) for Hex and *RigidRMSD* as a function of the RMSD threshold. Right: Average time spent on clustering docking solutions by Hex and *RigidRMSD* as a function of the RMSD threshold. For both plots, we chose five structures with the number of atoms in the ligand protein of about 2,000 such that they result in a similar number of clusters and plotted the standard deviation of the average cluster size (left) and the average clustering time (right) for these structures. For each protein complex, the number of considered docking solutions was fixed to 10,000.