Supplementary Information

"Combining the MARTINI and structure-based coarse-grained approaches for the molecular dynamics studies of conformational transitions in proteins"

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Discussion on the contact maps

Overlap criterion: According to the overlap criterion (OV), two amino acids will form a native contact if the Van der Waals spheres of any heavy atoms between different amino acids (close amino acids, with the sequential distance smaller than 4, are excluded) enhanced by the factor $(26/7)^{1/6}$ overlap. We provide the radii for each atom for each amino acid below [Tsai et al. J. Mol. Biol. 290, 253 (1999), Chwastyk et al. Proteins 84, 1275 (2016)]:

Table S1. Radii of heavy atoms for identifying contacts between amino acids according to the overlap criterion.

ATOM	R_{Tsai}	Notes
N Nη, Nε, Nζ, Nδ	1.64	Backbone and side chain in all amino acids
O	1.42	Backbone
Oγ	1.46	Side chain SER,THR
Oδ	1.46	Side chain ASP
Oε	1.42 1.46	Side chain GLN Side chain GLU
OH	1.46	Side chain TYR
Sδ	1.77	Side chain CYS,MET
C Cα Cβ Cγ	 1.88 1.88 1.88 1.61	 Backbone All amino acids except GLY LEU, ARG LEU, ARG, ILE and others
Cδ	1.88 1.76 1.61	PRO LYS,PRO, ARG and others LYS,PRO, ARG and others
Cε	1.88 1.76 1.61	LYS TRP, HIS TRP, HIS
Cζ	1.61 1.76	PHE TRP, TYR
Cη2	1.76	PHE, TRP, TYR

rCSU contacts: The rCSU contacts can be obtained from:
http://info.ifpan.edu.pl/~kwolek/rcsu/.
The rCSU contact map is an improved version of the original CSU contact map [V. Sobolev, R. C. Wade, G. Vriend, M. Edelman. Struct. Funct. Bioinf. 25, 120 (1996)] and has been discussed in [K. Wołek, A. Gómez-Sicilia, M. Cieplak, J. Chem. Phys. 143, 243105 (2015)].

The rCSU map distinguishes between the proper and destabilizing (repulsive "r") atomic contacts. According to this criterion, two amino acids are in contact when the number of proper atomic contacts is bigger than the number of destabilizing contacts. The rCSU contact map also identifies contacts of chemical nature, for example, ionic bridges. The definition of contacts in the rCSU algorithm and a server to run various examples can be found at http://info.ifpan.edu.pl/~kwolek/rcsu/.

Pulling results for 1AOH and 1UBQ proteins

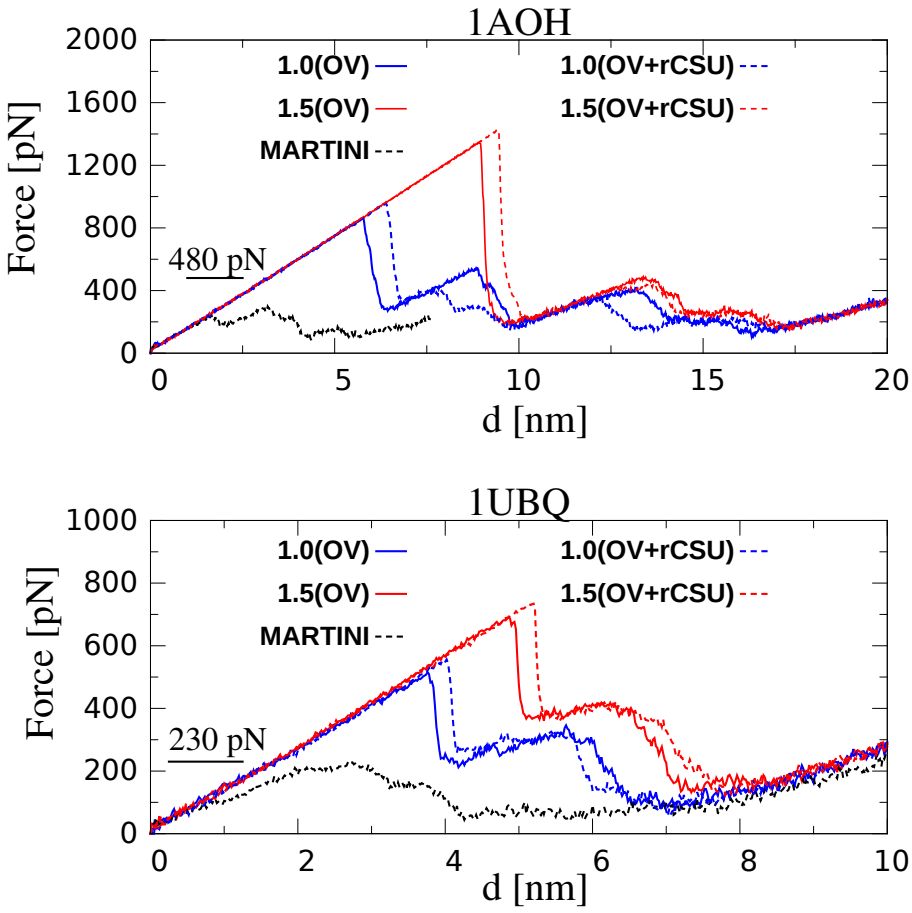

Figure S2. Results from pulling simulations for the 1AOH and 1UBQ cases, as indicated. A related discussion can be found in the "results" section of the article.

Substitution of harmonic bonds with Lennard—Jones interactions [ELNEDIN(1.5LJ)]

Figure S3 presents a comparison between the GoMARTINI based on the OV+rCSU contact map and the ELNEDIN approach with harmonic bonds being substituted with Lennard—Jones (LJ) interactions. The all-atom results and the original ELNEDIN results are also shown in figure S3 for the sake of comparison. The contact map is a key element for the dynamics of the native protein structures. The substitution of harmonic bonds with LJ interactions also has an impact on the results.

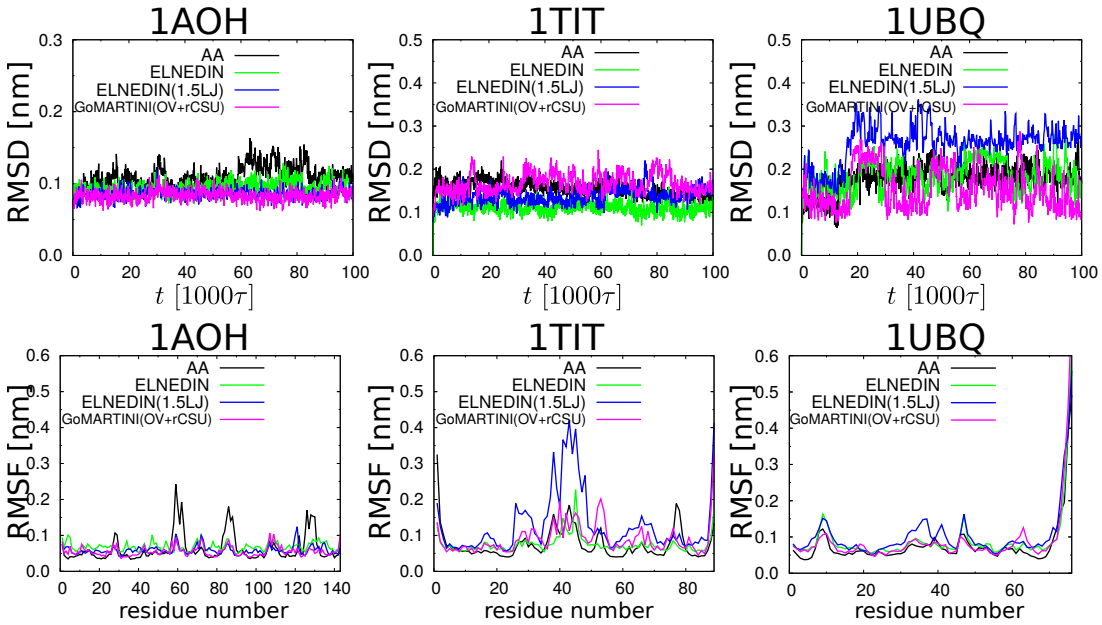

Figure S3. RMSD and RMSF for three proteins as indicated from AA (all-atom), ELNEDIN (EN based on harmonic bonds), ELNEDIN(1.5LJ) (ELNEDIN based on LJ potentials with λ=1.5), and GoMARTINI based on the OV+rCSU contact map with λ=1.5.

PCA for the RMSF of Man5B based on the OV contact map as obtained from the GoMARTINI

In figure S4 we present results based on the GoMARTINI approach and the OV contact map with λ=1.5. Results obtained from ELNEDIN and all-atom simulations are also shown. The GoMARTINI approach based on the OV contact map is able to capture the fluctuation of the catalytic pocket, but it also results in higher fluctuations in other parts of the protein (cf. figure 3 of the manuscript).

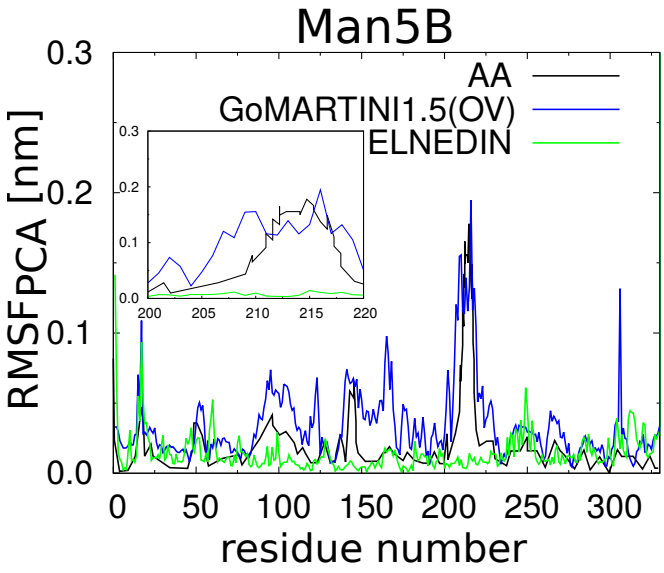

Figure S4. Principal Component Analysis of the RMSF for the C_α-atoms (AA) of the coarse-grained backbone beads (ELNEDIN and GoMARTINI) of the Man5B. We present results obtained from AA, ELNEDIN and GoMARTINI models based on the OV contact map with λ=1.5, as indicated. The AA data were taken from Figure 4 in [Bernardi et al., Biotechnol. Biofuels 7, 83 (2014)]) by using the g3data software. The inset shows the fluctuation from the catalytic region between the 200 and 220 amino acid residues in Man5B.

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