
Supporting Information for
Extension of the UNRES Coarse-Grained Force Field to Membrane
Proteins in the Lipid Bilayer

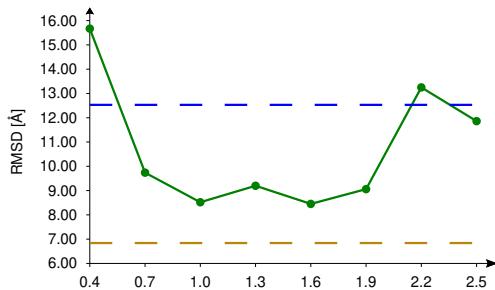
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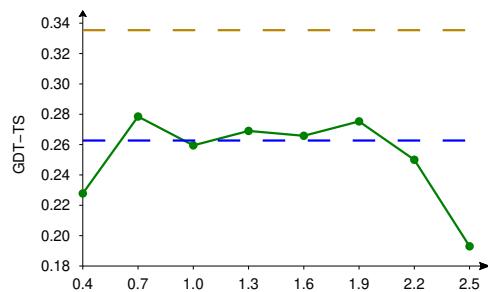
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adasko@sun1.chem.univ.gda.pl

Table S1. The lipid-phase well depths ($4\epsilon_L^\circ$; $kcal/mol$, lower triangle) and the water-phase well depths ($4\epsilon_w^\circ$; $kcal/mol$, upper triangle; data from Liwo et al., *J. Comput. Chem.*, **1997**, 18, 874-887) of the side-chain-interaction ($U_{SC_iSC_j}$) potentials.

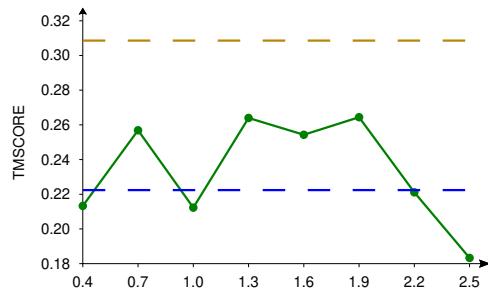
	Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala	Gly	Thr	Ser	Gln	Asn	Glu	Asp	His	Arg	Lys	Pro	
	5.605	6.220	6.216	6.439	6.210	5.960	5.431	4.879	5.264	5.496	4.293	4.358	4.267	3.681	3.541	3.703	4.718	3.381	3.794	4.516	Cys
		6.630	6.672	6.817	6.838	6.351	6.143	5.520	5.486	4.938	4.280	4.053	4.209	3.539	3.421	2.800	4.816	3.879	3.588	4.646	Met
Cys	2.252	6.642	6.972	6.924	6.529	6.139	5.442	5.291	4.788	4.130	3.941	3.902	3.608	3.081	3.018	4.794	3.871	3.683	4.487	4.902	Phe
Met	2.758	3.378	7.327	7.297	7.049	6.257	5.813	5.885	5.346	4.715	4.486	4.309	3.693	4.010	3.658	4.590	4.461	4.633	4.902	4.902	Ile
Phe	2.829	3.465	3.553	7.011	6.834	6.205	5.580	5.672	5.201	4.197	4.238	3.895	3.568	3.114	2.762	4.509	4.024	3.980	4.809	4.809	Leu
Ile	2.574	3.152	3.233	2.942	6.535	5.884	5.110	5.552	4.959	4.203	4.035	3.651	3.464	3.161	2.798	4.042	3.442	3.862	4.593	4.593	Val
Leu	2.574	3.152	3.233	2.942	2.942	5.283	4.830	4.758	4.725	3.566	3.561	3.927	3.766	3.586	3.552	4.651	4.242	4.099	4.508	4.508	Trp
Val	2.314	2.835	2.907	2.645	2.645	2.378	4.222	4.163	3.979	3.162	2.938	3.137	2.803	2.658	2.873	3.879	3.444	3.441	4.092	4.092	Tyr
Trp	3.329	4.077	4.182	3.805	3.805	3.421	4.921	4.386	3.652	3.026	2.568	2.500	2.139	1.471	1.737	3.105	2.015	1.820	3.640	3.640	Ala
Tyr	3.124	3.826	3.924	3.570	3.570	3.210	4.618	4.333	2.502	2.788	2.142	1.074	1.324	-0.271	0.761	2.863	1.500	-0.239	3.538	3.538	Gly
Ala	1.679	2.057	2.109	1.919	1.919	1.726	2.482	2.329	1.252	2.290	2.247	1.505	1.403	0.968	1.308	2.860	1.983	-0.009	2.956	2.956	Thr
Gly	1.245	1.525	1.564	1.423	1.423	1.280	1.841	1.728	0.929	0.689	1.280	0.769	0.912	-0.074	0.367	2.429	1.499	-0.213	2.942	2.942	Ser
Thr	2.418	2.961	3.037	2.763	2.763	2.484	3.574	3.353	1.803	1.337	2.595	-0.679	0.453	-0.759	-0.362	1.680	0.678	-0.535	2.621	2.621	Gln
Ser	2.139	2.619	2.686	2.444	2.444	2.198	3.161	2.966	1.595	1.183	2.296	2.031	0.414	-0.164	0.221	2.129	0.390	-0.235	2.326	2.326	Asn
Gln	2.903	3.556	3.646	3.318	3.318	2.983	4.291	4.027	2.164	1.605	3.116	2.757	3.742	-3.519	-2.016	1.836	2.749	2.010	1.798	1.798	Glu
Asn	2.676	3.277	3.361	3.058	3.058	2.750	3.955	3.711	1.995	1.480	2.872	2.541	3.449	3.179	-1.353	2.550	2.820	1.625	1.863	1.863	Asp
Glu	2.916	3.572	3.663	3.333	3.333	2.997	4.311	4.045	2.174	1.613	3.131	2.769	3.759	3.465	3.776	3.729	2.294	-0.030	3.112	3.112	His
Asp	2.690	3.295	3.379	3.074	3.074	2.764	3.977	3.731	2.006	1.481	2.888	2.554	3.468	3.196	3.483	3.213	-0.083	-1.604	2.444	2.444	Arg
His	2.935	3.594	3.686	3.354	3.354	3.016	4.338	4.071	2.188	1.623	3.150	2.787	3.783	3.487	3.800	3.505	3.824	-4.390	2.366	2.366	Lys
Arg	3.360	4.116	4.221	3.840	3.840	3.453	4.967	4.661	2.505	1.858	3.607	3.191	4.331	3.992	4.351	4.014	4.379	5.014	4.193	4.193	Pro
Lys	2.905	3.558	3.649	3.320	3.320	2.985	4.294	4.030	2.166	1.607	3.118	2.759	3.745	3.451	3.761	3.470	3.785	4.334	3.747	3.747	
Pro	2.252	2.759	2.829	2.574	2.574	2.315	3.330	3.124	1.679	1.246	2.418	2.139	2.903	2.676	2.917	2.690	2.935	3.361	2.905	2.253	



A

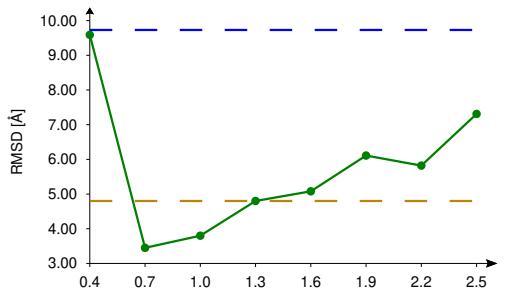


B

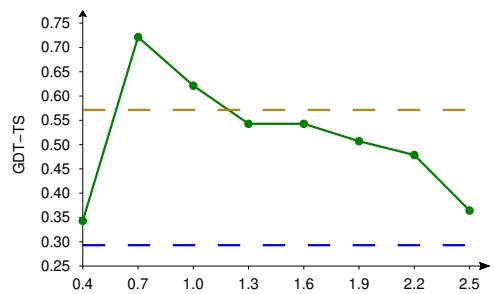


C

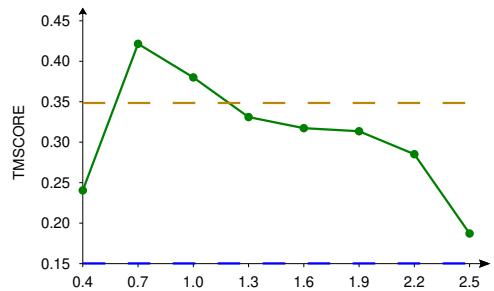
Figure S1. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1A91 obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

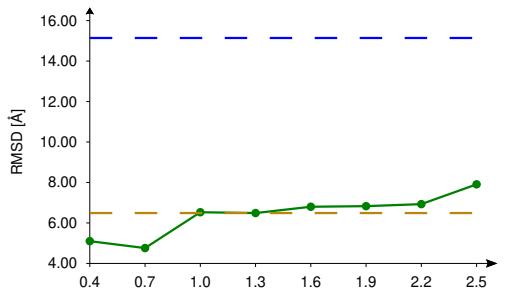


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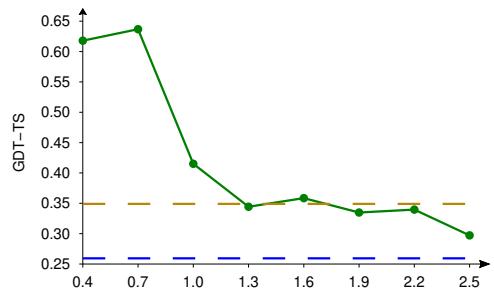


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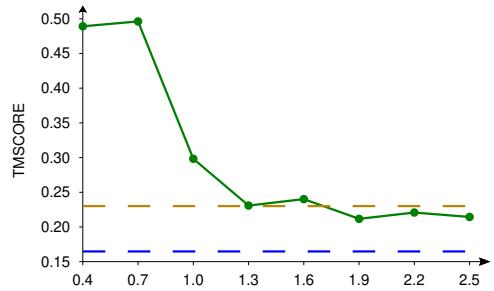
Figure S2. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1IIJ obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

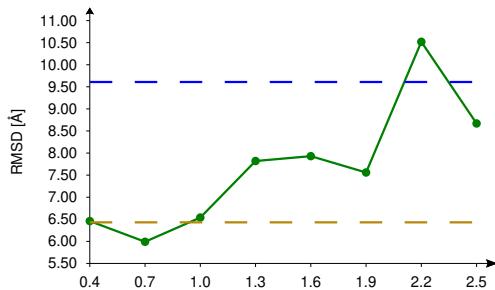


B

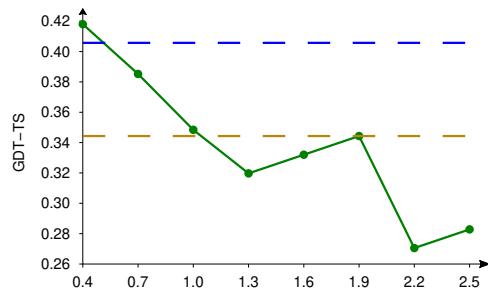


C

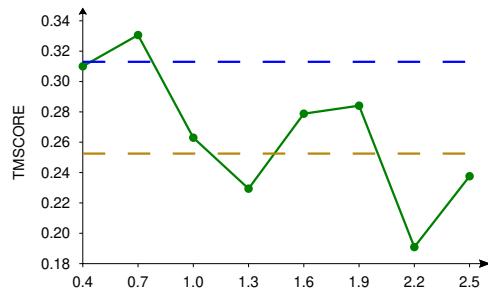
Figure S3. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1N71 obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A



B



C

Figure S4. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1VRY obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.

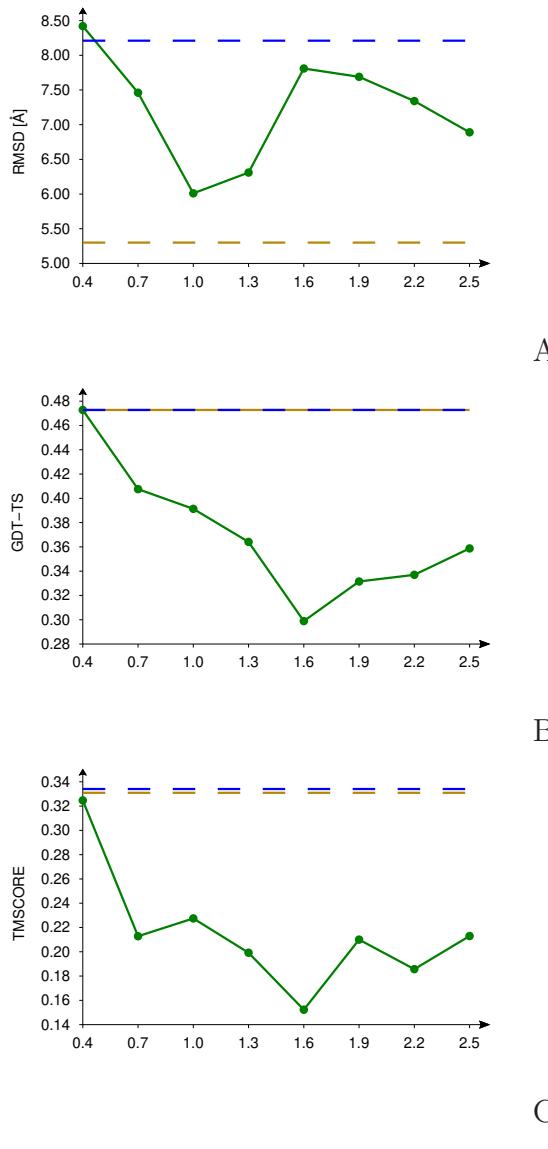
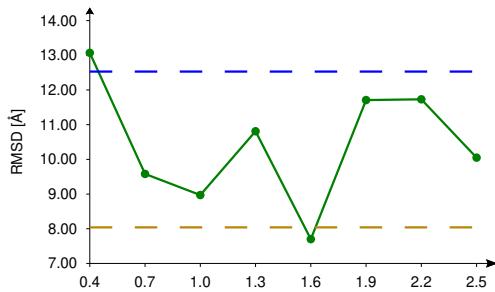
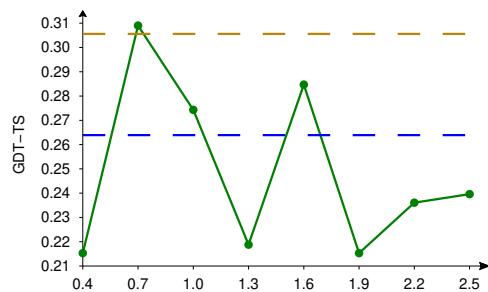


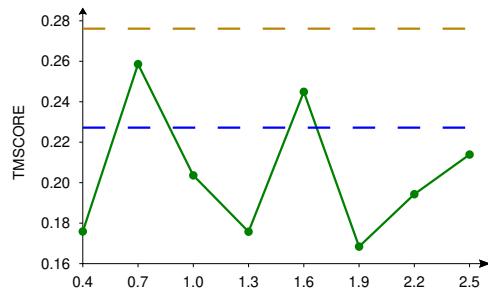
Figure S5. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1WAZ obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

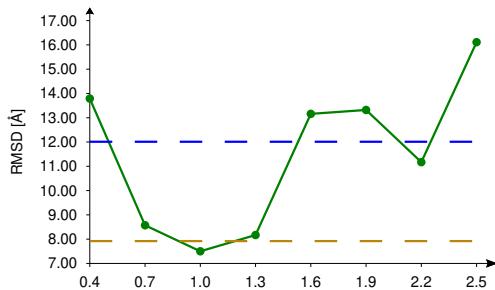


B

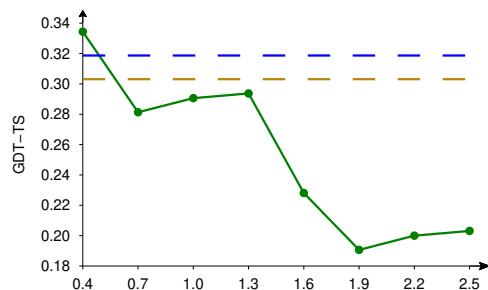


C

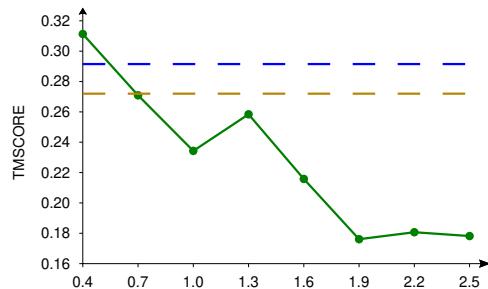
Figure S6. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 1WU0 obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

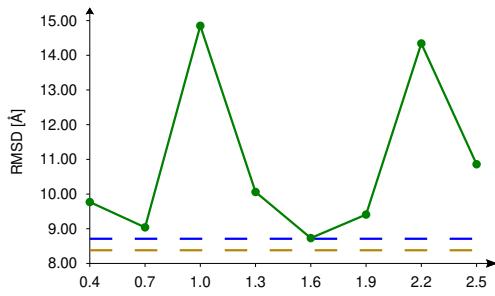


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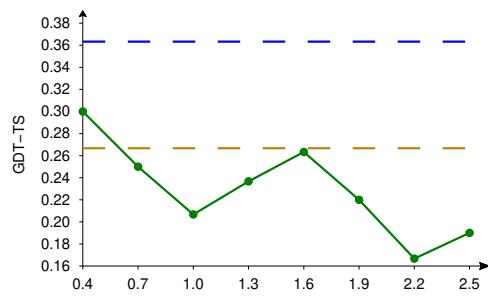


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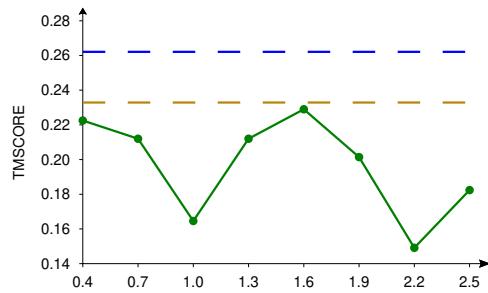
Figure S7. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 2K9P obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

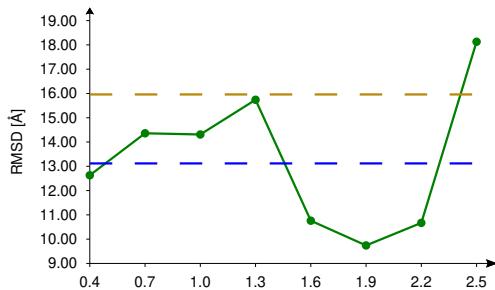


B

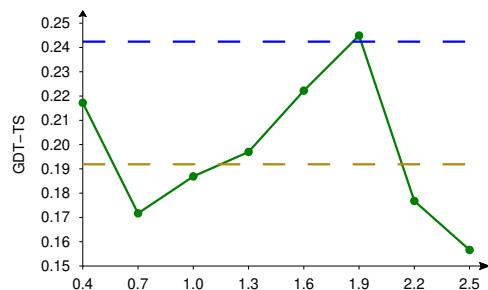


C

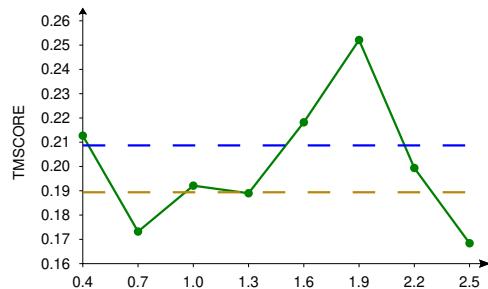
Figure S8. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 2KSD obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A

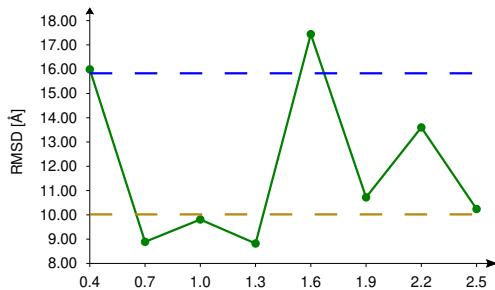


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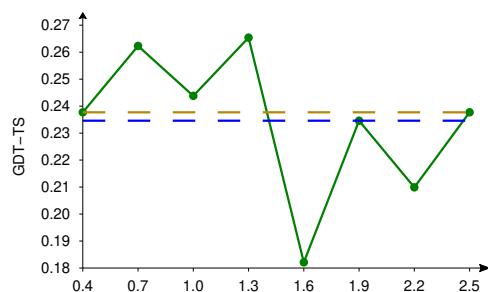


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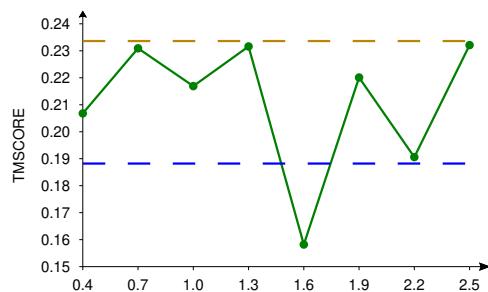
Figure S9. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 2LOP obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.



A



B



C

Figure S10. Plots of RMSD (A), GDT_TS (B), and TM-score (C) as functions of the s_L parameter (eq 9 of the main text) of the lowest-RMSD family of conformations of 2MOZ obtained with $\Delta G_{p_i} = 0$ kcal/mol. The values corresponding to all-water and all-lipid environments are as yellow and blue dashed lines respectively.

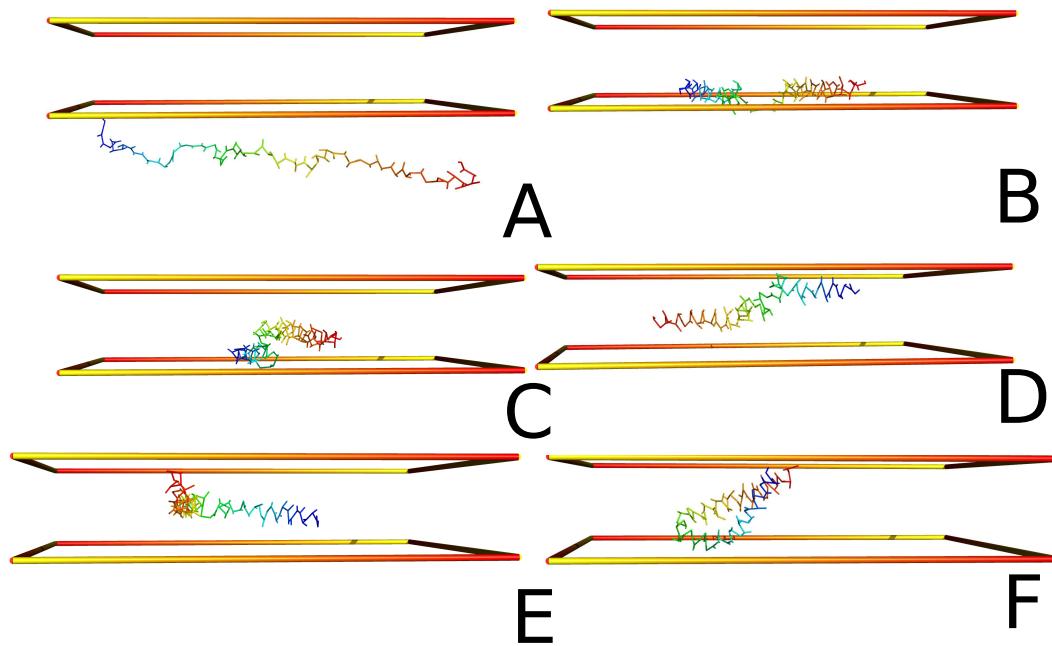


Figure S11. Snapshots from a trajectory of the 1A91 protein simulated folding.

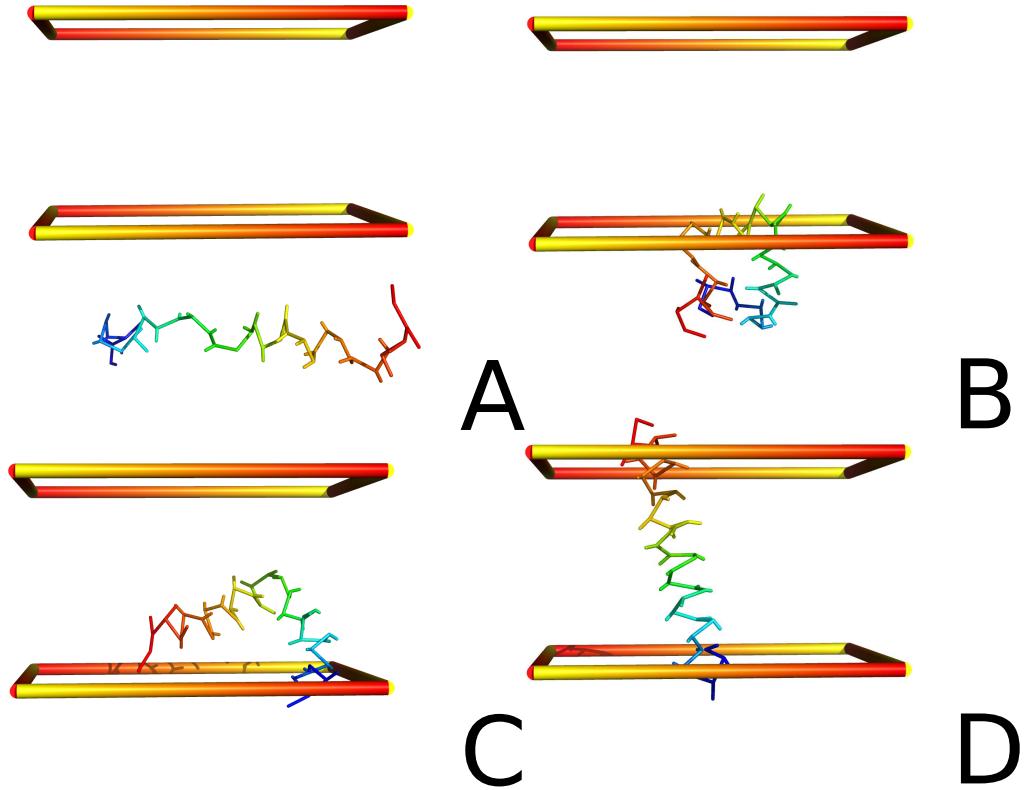


Figure S12. Snapshots from a trajectory of the 1IIJ protein simulated folding.

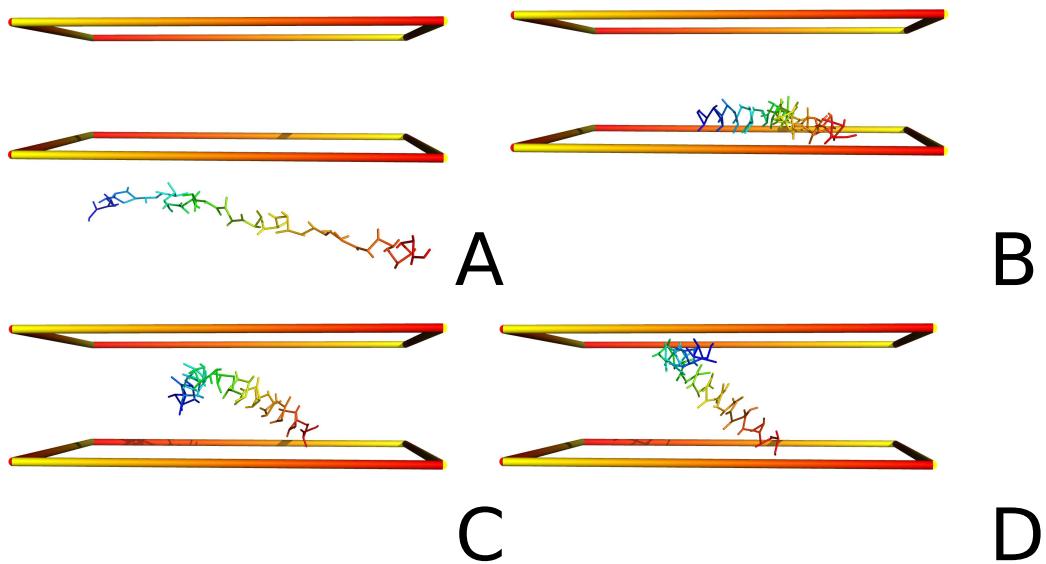


Figure S13. Snapshots from a trajectory of the 1N7L protein simulated folding.

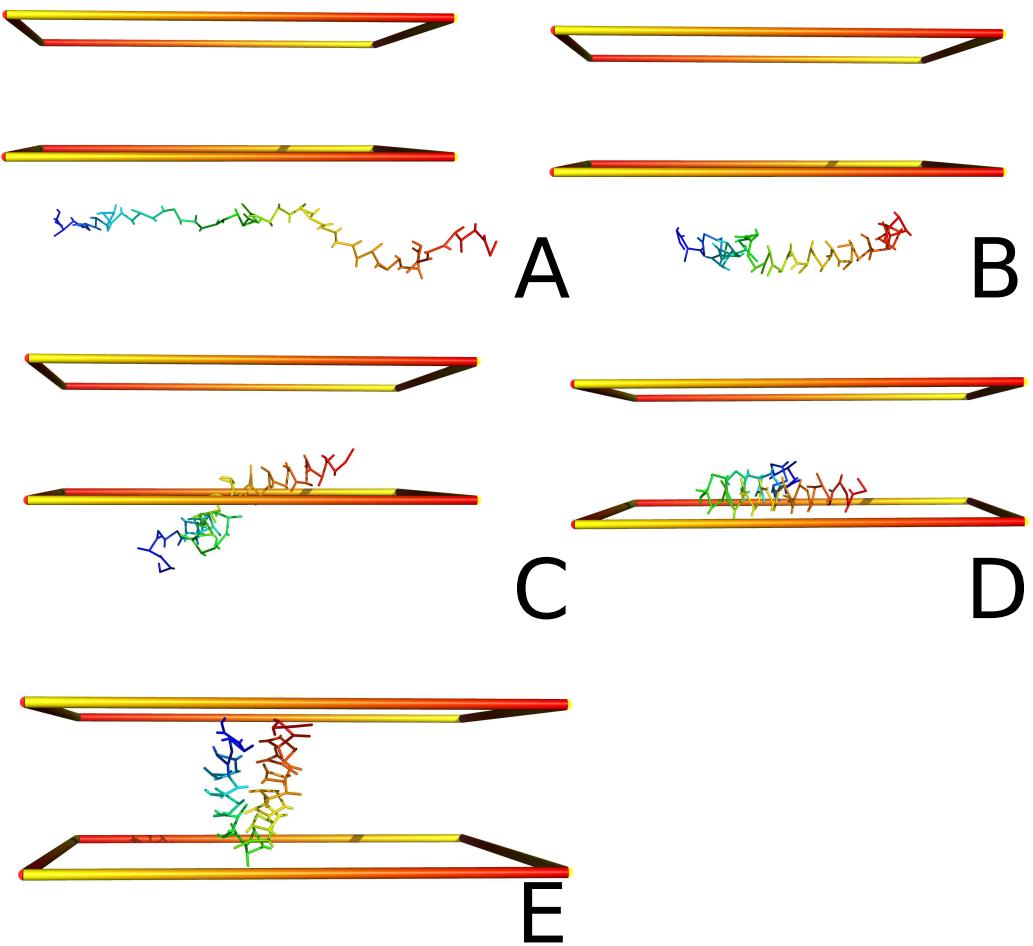


Figure S14. Snapshots from a trajectory of the 1VRY protein simulated folding.

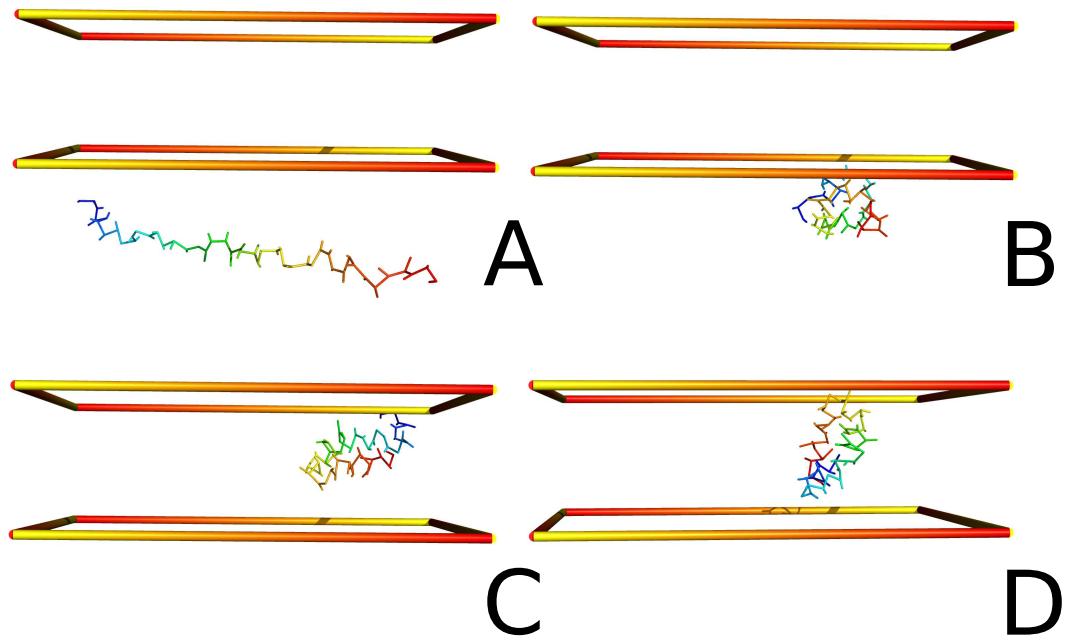


Figure S15. Snapshots from a trajectory of the 1WAZ protein simulated folding.

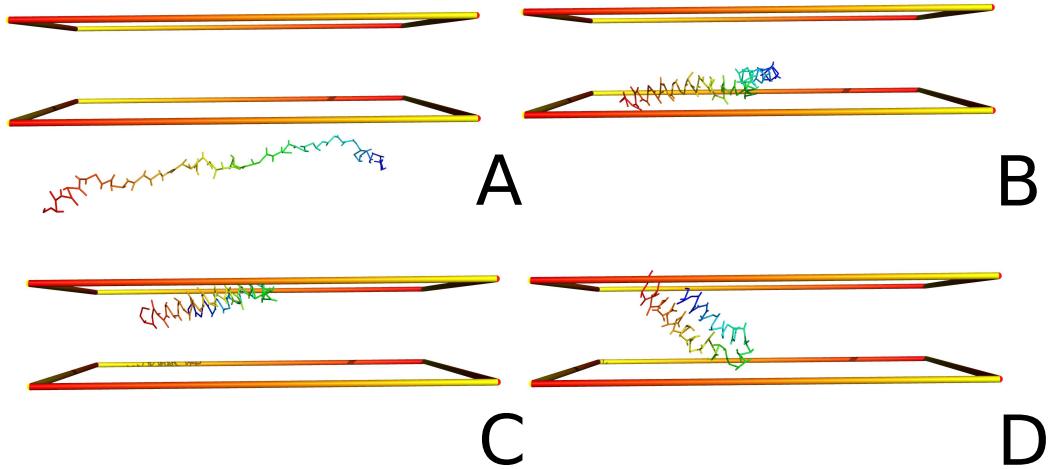


Figure S16. Snapshots from a trajectory of the 1WU0 protein simulated folding.

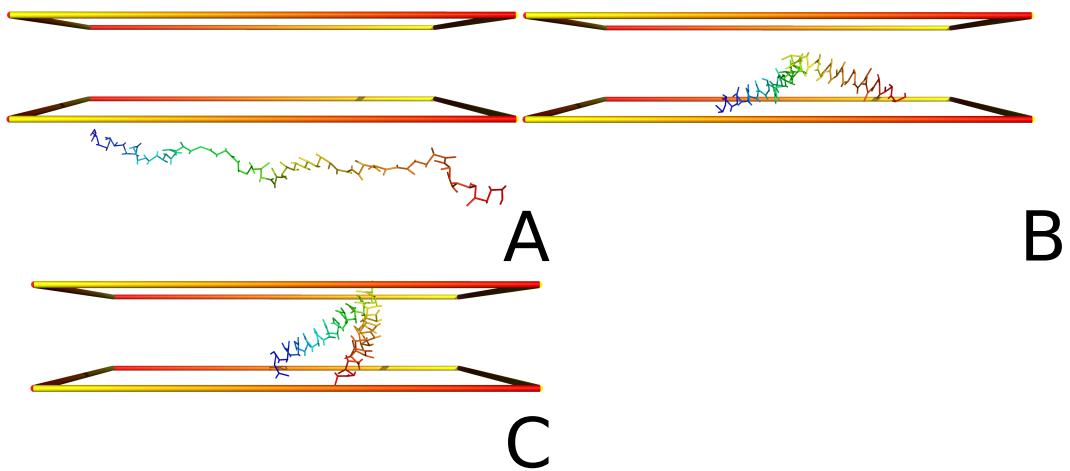


Figure S17. Snapshots from a trajectory of the 2K9P protein simulated folding.

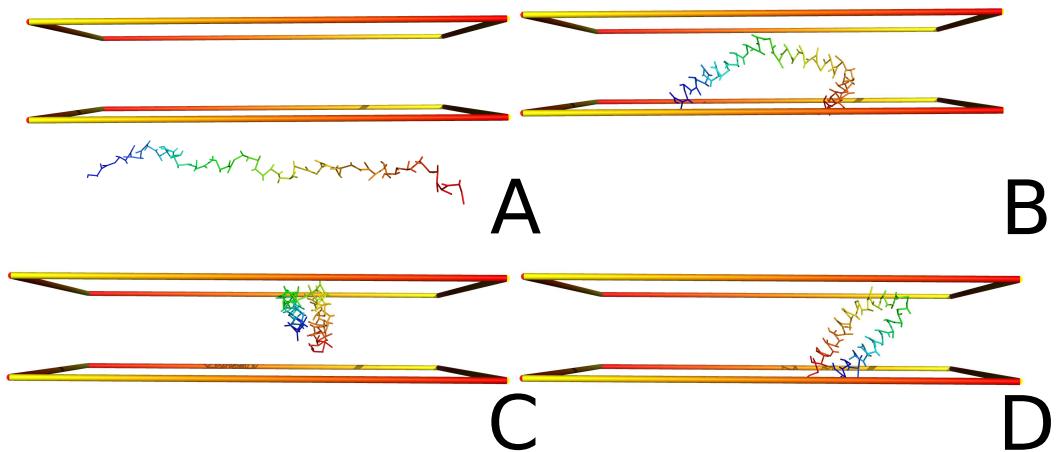


Figure S18. Snapshots from a trajectory of the 2KSD protein simulated folding.

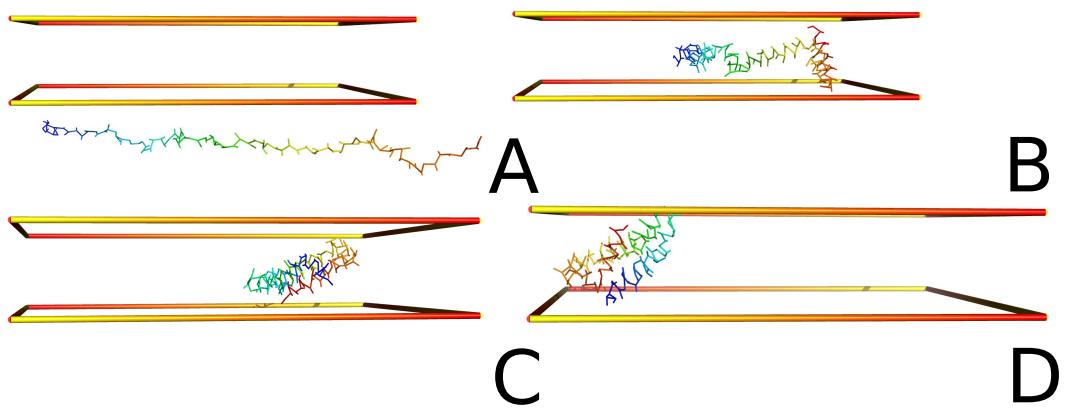


Figure S19. Snapshots from a trajectory of the 2LOP protein simulated folding.

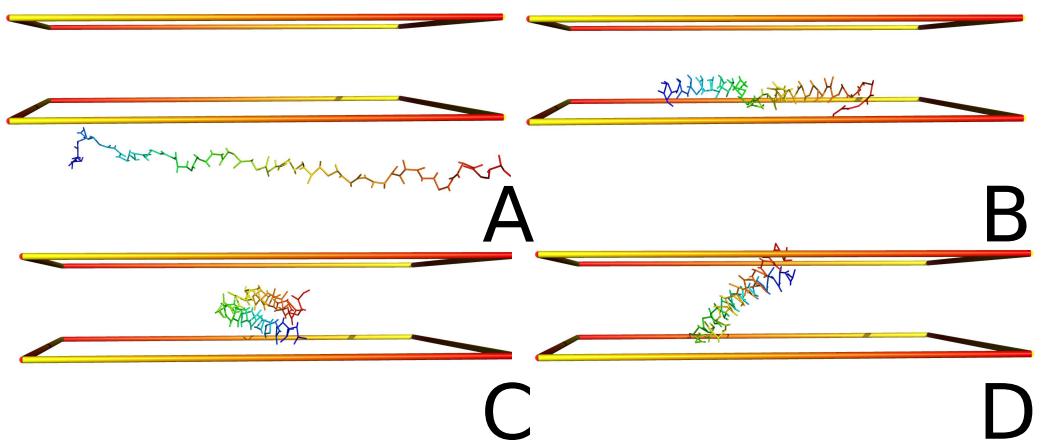


Figure S20. Snapshots from a trajectory of the 2MOZ protein simulated folding.