Supporting Information for: Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics

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Table S1: Parameters of $U^{(3)}_{corr}$ and $U^{(3)}_{turn}$ of eq. (1) (in [kcal/mol]), which are the coefficients of the second-order Fourier expansion of the energy surfaces of terminally-blocked glycine, L-alanine, and L-proline, respectively [see eqs. (23-28), (43), (44), and (46) of ref. 17 for definition].

	FF1/FF2/OPT-W			OPT-WTF			OPT-WTFSA-1			OPT-WTFSA-2			OPT-ALL		
coefficient	Gly	Ala	Pro	Gly	Ala	Pro	Gly	Ala	Pro	Gly	Ala	Pro	Gly	Ala	Pro
b_{11}	0.20607	-0.23379	0.03181	0.21284	-0.19527	-0.43107	0.21622	-0.18616	-0.34521	0.15477	-0.15504	-0.52839	0.18487	-0.16894	-0.34638
b_{12}	0	-1.50122	-1.01539	0	-1.49695	-0.58867	0	-1.21868	-0.53032	0	-0.87734	-0.73455	0	-1.30274	-0.65691
b_{21}	0.79197	0.50026	-1.28648	0.29196	0.287	-0.78683	0.29227	0.25008	-0.78799	0.07024	0.16261	-0.28972	0.29198	0.30877	-0.84702
b_{22}	0	-0.87802	-0.90663	0	-0.60307	-1.40378	0	-0.50469	-1.11152	0	-0.37918	-1.23898	0	-0.55941	-1.28025
c_{11}	-0.92796	2.30237	1.91437	-0.92796	2.30237	1.91437	-0.92796	2.30237	1.91437	-0.92796	2.30237	1.91437	-0.92796	2.30237	1.91437
c_{12}	0	-1.59642	-0.45484	0	-1.59642	-0.45484	0	-1.59642	-0.45484	0	-1.59642	-0.45484	0	-1.59642	-0.45484
d_{11}	2.37346	-2.08973	-1.54887	2.37346	-2.08973	-1.54887	2.37346	-2.08973	-1.54887	2.37346	-2.08973	-1.54887	2.37346	-2.08973	-1.54887
d_{12}	0	-0.5325	0.66414	0	-0.5325	0.66414	0	-0.5325	0.66414	0	-0.5325	0.66414	0	-0.5325	0.66414
e_{11}	0.95884	1.67624	0.05189	1.03054	1.57762	0.8266	0.95578	1.44523	0.79551	0.78368	1.23838	0.98629	1.04848	1.56514	1.00834
e_{12}	0	-0.1433	0.36165	0	-0.4094	0.63668	0	-0.37727	0.54228	0	-0.34181	0.20093	0	-0.38226	0.4694
e_{21}	0	-0.94426	0.27109	0	-0.89626	0.27244	0	-0.82147	0.08132	0	-0.72205	-0.14635	0	-0.91296	-0.08638
e_{22}	-1.7	-0.87636	0.15447	-1.95114	-1.19958	-0.07082	-1.77486	-1.09585	-0.10191	-1.63054	-0.96776	-0.05061	-1.92606	-1.16158	0.1951

Table S2: Parameters of the torsional potentials.[a]

Gly-Gly	FF1/FF2/OPT-W		OPT-WTF		OPT-WTFSA-1		OPT-WTFSA-2		OPT-ALL	
n	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}
1	4.03053E-03	0.00000E+00	2.42744E-01	0.00000E+00	2.91221E-01	0.00000E+00	3.89266E-01	0.00000E+00	1.74301E-01	0.00000E+00
2	-4.90330E-03	0.00000E+00	1.26123E-01	0.00000E+00	1.97221E-01	0.00000E+00	4.18662E-01	0.00000E+00	1.70239E-01	0.00000E+00
3	2.70952E-01	0.00000E+00	1.09661E-02	0.00000E+00	3.47215E-02	0.00000E+00	-4.85875E-03	0.00000E+00	9.59526E-02	0.00000E+00
4	-7.20927E-02	0.00000E+00	-8.38956E-02	0.00000E+00	-1.25868E-01	0.00000E+00	-2.28912E-01	0.00000E+00	-3.30271E-03	0.00000E+00
5	-3.66258E-03	0.00000E+00	-7.53949E-02	0.00000E+00	-8.07275E-02	0.00000E+00	-1.32435E-01	0.00000E+00	-3.18402E-02	0.00000E+00
6	-6.34294E-03	0.00000E+00	-9.04322E-03	0.00000E+00	-3.07820E-03	0.00000E+00	-3.25567E-02	0.00000E+00	-6.62775E-02	0.00000E+00
Gly-Ala										
1	1.27465E-02	-1.01763E-01	1.28060E-01	-1.28448E-01	1.37258E-01	-1.87823E-01	4.48732E-01	-6.17446E-01	1.60453E-01	-1.60717E-01
2	-8.41985E-03	1.18716E-02	2.66837E-03	-7.72357E-02	-3.24314E-03	-1.14115E-01	-7.19420E-02	-2.81509E-01	-2.07481E-02	-1.34295E-01
3	2.50582E-01	3.30235E-02	7.45075E-02	3.52903E-02	1.00886E-01	6.20938E-02	8.55553E-02	9.54595E-02	7.48213E-02	2.87069E-02
4	-1.02631E-01	1.46337E-01	-6.39584E-02	1.20525E-01	-1.24448E-01	1.61747E-01	-1.78171E-01	2.81875E-01	-8.92972E-02	1.64413E-01
5	6.63161E-03	8.86275E-03	-1.44598E-02	7.72427E-02	-1.22389E-02	1.29629E-01	-3.35660E-02	2.20930E-01	-2.97479E-02	-1.50259E-02
6	-6.81049E-03	8.71641E-03	3.18274E-02	-3.69001E-02	1.18244E-02	-7.32819E-02	7.48948E-02	-1.48385E-01	5.60675E-02	-2.40954E-02
Gly-Pro										
1	-1.14953E+00	1.29720E+00	-1.04396E-01	3.29131E-01	-2.35280E-01	4.47825E-01	-1.02764E+00	7.71574E-01	-3.08965E-01	4.71873E-01
2	-1.08859E-03	-1.20321E-02	1.79606E-01	3.28557E-01	2.25332E-01	4.39143E-01	6.60187E-01	4.73949E-01	2.80245E-01	2.29029E-01
3	4.04229E-01	2.92750E-01	1.70178E-02	-2.30205E-02	8.54137E-02	-3.13391E-02	3.06766E-01	6.26077E-02	9.36645E-02	-2.92251E-02
4	-2.41994E-01	5.38295E-02	3.05967E-02	-4.34448E-02	9.34821E-04	-5.34886E-03	1.12028E-01	-2.20307E-03	8.55039E-02	5.20027E-02
5	4.31804E-02	-6.56306E-02	1.30312E-01	2.49787E-01	1.29469E-01	2.38018E-01	1.41205E-01	4.63242E-01	2.64316E-02	2.37259E-01
6	4.29080E-02	1.38685E-01	-2.51201E-01	2.85415E-02	-1.67401E-01	1.36767E-01	-2.32839E-01	2.16374E-01	-9.24990E-02	8.79232E-03
7	-6.31286E-02	-2.65338E-02	1.17569E-01	-1.07719E-01	-9.09952E-03	-1.50380E-01	4.45175E-02	-2.13921E-01	3.55825E-02	-1.79600E-02
8	1.46743E-02	-3.26658E-03	6.81505E-02	3.28407E-02	1.59178E-01	1.58505E-02	2.13415E-01	1.05584E-01	1.06302E-01	4.57412E-02
9	-1.33460E-02	3.01470E-02	-7.16768E-02	4.70660E-02	-5.07021E-02	9.02235E-02	-1.06794E-01	1.83807E-01	-2.54232E-02	2.22427E-02
10	-1.11258E-02	-3.15723E-02	9.24555E-03	-5.50703E-03	-2.74002E-02	3.70860E-02	-1.58917E-01	-4.77027E-02	-5.14340E-03	6.30619E-02

[a] The torsional potential is expressed by $U_{tor}(\gamma) = \sum_{n=1}^{N} V_{1n}[1+\cos(n\gamma)] + V_{2n}[1+\sin(n\gamma)]$, where N is the order of the expansion (6 for paird of residues not containing proline and 10 for the pairs containing proline).

Table S2 (continued)

Ala-Gly	FF1/FF2/OPT-W		OPT-WTF		OPT-WTFSA-1		OPT-WTFSA-2		OPT-ALL	
n	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}
1	5.14830E-03	9.48478E-02	-1.56521E-01	6.58654E-02	-2.29844E-01	8.10157E-02	-5.35331E-01	3.07619E-01	-2.18510E-01	8.75036E-02
2	-8.85552E-02	1.20661E-01	-5.62095E-02	4.47746E-02	-7.16965E-02	8.72173E-02	-4.40634E-03	2.42563E-01	-3.68971E-02	9.08331E-02
3	2.65903E-01	-8.99192E-02	2.48133E-01	-2.88012E-02	3.14208E-01	-5.35383E-02	4.08626E-01	-1.26381E-01	2.03230E-01	-2.96330E-02
4	-6.16552E-02	-6.07952E-02	-1.36776E-01	-5.18567E-02	-2.02452E-01	-6.71549E-02	-3.75632E-01	-1.24731E-01	-1.44691E-01	-7.35262E-02
5	2.19209E-02	-3.09487E-02	4.58441E-02	-2.15490E-02	6.37359E-02	-3.21902E-02	1.54159E-01	-4.34413E-02	5.29656E-02	-3.45087E-02
6	-1.58136E-02	-1.74252E-02	2.77368E-02	-2.68518E-02	1.20409E-02	-4.77091E-02	-5.10726E-03	-8.98940E-02	-2.96936E-03	-3.30624E-02
Ala-Ala										
1	1.05084E+00	-1.83406E-03	3.86474E-01	7.04576E-02	4.84934E-01	1.01827E-01	7.57412E-01	2.41619E-01	3.66217E-01	6.87184E-02
2	2.56198E-01	3.75825E-02	1.49080E-01	-9.30279E-02	2.02908E-01	-1.57752E-01	3.16517E-01	-4.83719E-01	1.52696E-01	-1.10376E-01
3	2.97224E-01	-6.65886E-03	1.25835E-01	3.20767E-04	1.83892E-01	-9.11332E-03	2.94869E-01	-3.00853E-02	1.37689E-01	-1.25909E-02
4	-9.30144E-02	2.78499E-02	-2.69167E-02	2.85179E-02	-5.50573E-02	3.62865E-02	-1.18430E-01	6.30789E-02	-4.87958E-02	2.52107E-02
5	2.69127E-02	-2.79813E-03	1.15945E-02	1.96771E-02	2.01397E-02	1.58844E-02	1.39669E-02	6.86930E-02	4.33588E-03	1.02044E-02
6	-5.69348E-03	-5.76679E-03	4.83891E-03	3.01462E-03	6.37922E-03	2.45381E-03	5.15960E-03	2.89140E-02	3.89350E-03	6.42890E-04
Ala-Pro										
1	1.97348E+00	3.61809E+00	2.84232E-01	1.40684E+00	1.05440E+00	1.99420E+00	1.24599E+00	3.28913E+00	5.21295E-01	1.63964E+00
2	3.25172E-01	6.93324E-01	-1.83643E-01	7.30930E-03	4.15367E-01	2.58231E-01	3.71946E-01	6.21240E-01	-1.46616E-01	5.02152E-01
3	7.44811E-01	2.28853E-01	1.60514E-01	4.07847E-02	4.38811E-01	1.78360E-01	1.72894E-01	5.10551E-01	-1.54361E-01	2.90871E-01
4	-1.11515E-02	4.21766E-01	-3.32488E-01	2.12639E-01	-6.03233E-02	1.44596E-01	-4.30010E-01	1.34074E-01	-3.65292E-01	1.77057E-01
5	-1.09160E-01	4.09945E-02	-3.83146E-01	-2.20326E-01	-1.32748E-01	-8.30658E-02	-1.04165E-01	-1.24492E-01	-3.11814E-01	5.61404E-02
6	1.08618E-01	6.71048E-03	8.66138E-02	-1.56685E-01	7.92515E-02	-1.23210E-01	1.84767E-01	1.76351E-01	-2.45790E-01	6.92134E-02
7	1.21785E-02	9.37813E-02	-1.80020E-02	1.14932E-01	1.46959E-01	9.69035E-02	9.14037E-02	1.45966E-01	-1.15288E-01	5.57365E-02
8	-2.77282E-02	2.84981E-02	-1.36034E-01	-1.53133E-02	-8.27696E-02	2.19985E-01	2.88613E-01	2.65632E-01	-8.75484E-02	3.85364E-01
9	2.15879E-02	1.85528E-02	-4.24074E-02	-8.96885E-02	-2.20971E-01	9.42558E-04	-5.37851E-02	5.01514E-01	-4.72782E-01	2.90614E-01
10	-8.56980E-03	3.92482E-02	2.78082E-02	-1.77286E-02	-2.11828E-02	-3.91532E-02	-2.33602E-01	1.43541E-01	-2.67882E-01	-6.87347E-02

Table S2 (continued)

Pro-Gly	FF1/FF2/OPT-W		OPT-WTF		OPT-WTFSA-1		OPT-WTFSA-2		OPT-ALL	
n	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}	V_{1n}	V_{2n}
1	2.12359E-02	4.05506E-02	2.12359E-02	4.05506E-02	2.12359E-02	4.05506E-02	2.12359E-02	4.05506E-02	2.12359E-02	4.05506E-02
2	-1.19424E-01	2.91087E-01	-1.19424E-01	2.91087E-01	-1.19424E-01	2.91087E-01	-1.19424E-01	2.91087E-01	-1.19424E-01	2.91087E-01
3	3.81770E-01	-1.11839E-01	3.81770E-01	-1.11839E-01	3.81770E-01	-1.11839E-01	3.81770E-01	-1.11839E-01	3.81770E-01	-1.11839E-01
4	-9.75339E-02	-7.60089E-02	-9.75339E-02	-7.60089E-02	-9.75339E-02	-7.60089E-02	-9.75339E-02	-7.60089E-02	-9.75339E-02	-7.60089E-02
5	-5.00214E-02	3.42037E-02	-5.00214E-02	3.42037E-02	-5.00214E-02	3.42037E-02	-5.00214E-02	3.42037E-02	-5.00214E-02	3.42037E-02
6	8.12296E-02	3.98713E-02	8.12296E-02	3.98713E-02	8.12296E-02	3.98713E-02	8.12296E-02	3.98713E-02	8.12296E-02	3.98713E-02
7	-1.21613E-02	-4.57682E-02	-1.21613E-02	-4.57682E-02	-1.21613E-02	-4.57682E-02	-1.21613E-02	-4.57682E-02	-1.21613E-02	-4.57682E-02
8	6.95870E-03	2.28245E-02	6.95870E-03	2.28245E-02	6.95870E-03	2.28245E-02	6.95870E-03	2.28245E-02	6.95870E-03	2.28245E-02
9	2.02598E-02	-2.00100E-02	2.02598E-02	-2.00100E-02	2.02598E-02	-2.00100E-02	2.02598E-02	-2.00100E-02	2.02598E-02	-2.00100E-02
10	-1.48685E-02	-1.09627E-02	-1.48685E-02	-1.09627E-02	-1.48685E-02	-1.09627E-02	-1.48685E-02	-1.09627E-02	-1.48685E-02	-1.09627E-02
Pro-Ala										
1	1.40539E+00	-7.42879E-01	-3.20533E-01	3.15921E-02	-5.30371E-01	-3.79838E-03	-1.44568E+00	4.48810E-01	-3.96444E-01	6.13025E-02
2	9.21075E-02	-1.17205E-01	1.13554E-01	-5.19080E-02	6.32663E-02	-1.09521E-01	2.44809E-01	-9.84525E-02	-4.09079E-02	6.58324E-02
3	4.49479E-01	3.82888E-02	9.07158E-02	1.47598E-02	1.21519E-01	8.43223E-03	7.10743E-02	-7.82747E-02	1.71063E-01	3.98565E-02
4	8.11975E-02	-3.35594E-02	2.79386E-03	6.10167E-02	-7.80575E-03	3.76829E-02	6.10521E-02	1.26535E-01	-1.52999E-02	5.11478E-02
5	-9.88964E-03	-4.63759E-02	-2.89267E-02	-1.49482E-02	-4.82717E-02	-4.37033E-02	-1.06073E-01	-5.66209E-02	-4.06339E-02	1.88726E-03
6	8.58396E-02	4.22362E-02	-1.14925E-02	7.55638E-02	-1.47599E-02	9.06497E-02	-2.54567E-02	1.39995E-01	1.29087E-02	1.53715E-02
7	2.73049E-02	-5.43392E-02	7.36475E-03	-1.06133E-03	4.59200E-02	2.27528E-02	8.12043E-02	4.96622E-02	3.72639E-02	2.52414E-02
8	-4.18620E-03	-1.04889E-02	-4.85280E-02	1.28637E-02	-7.44594E-02	4.24939E-02	-1.02693E-01	2.65604E-02	-4.19398E-02	-1.57948E-02
9	1.06804E-02	-7.89066E-03	-4.18452E-02	-3.58610E-02	-4.90352E-02	-2.08349E-02	-4.64168E-02	-6.09468E-02	-4.55500E-02	-8.28557E-02
10	-5.01879E-03	-1.20569E-02	-7.04322E-02	-2.28699E-02	-8.46346E-02	-1.07298E-02	-1.28754E-01	-4.35563E-02	-2.36828E-02	-5.73216E-02
Pro-Pro										
1	4.23219E+00	1.42318E+00	4.99990E+00	6.57351E-01	4.23486E+00	7.87119E-01	4.99994E+00	1.02894E+00	4.99465E+00	1.64599E+00
2	1.24967E+00	-2.32575E-01	2.68153E+00	2.35582E-01	2.59217E+00	-3.33044E-01	3.01919E+00	-1.08282E+00	2.80924E+00	1.41994E+00
3	5.38690E-01	-4.25507E-01	4.64903E-01	3.80079E-01	1.24864E+00	-4.98088E-01	1.44640E+00	-1.36232E+00	7.06830E-01	1.66781E+00
4	4.01096E-01	-6.42186E-01	-1.48440E+00	5.38356E-01	1.16294E-01	-1.79001E-01	1.53375E-01	-8.06450E-01	-1.48370E+00	1.78501E+00
5	2.52852E-01	-2.32257E-01	-3.01231E+00	5.03150E-01	-9.55402E-01	1.83034E-01	-1.13926E+00	-2.92452E-01	-3.06976E+00	1.65664E+00
6	-3.06406E-02	-2.48617E-01	-4.04831E+00	2.72333E-01	-1.87536E+00	2.47282E-01	-2.18888E+00	-1.79960E-01	-3.92308E+00	1.33325E+00
7	-1.68086E-02	-1.55069E-01	-4.34538E+00	3.10840E-01	-2.44663E+00	5.47506E-01	-2.71687E+00	2.89616E-01	-4.05289E+00	9.27957E-01
8	-9.68421E-02	-1.80718E-01	-3.59576E+00	5.24012E-01	-2.27142E+00	8.14203E-01	-2.52591E+00	9.09040E-01	-3.18681E+00	7.12034E-01
9	-2.73541E-02	-1.36915E-01	-2.06869E+00	5.47357E-01	-1.33942E+00	7.88906E-01	-1.45928E+00	1.12958E+00	-1.84067E+00	6.36232E-01
10	-6.08829E-02	-6.71426E-02	-6.17367E-01	1.76267E-01	-4.40969E-01	2.69137E-01	-4.89916E-01	3.69826E-01	-6.07914E-01	1.45237E-01

Table S3: Short ($\sigma^{\perp}$) and long axes ($\sigma^{\parallel}$), well-depth anisotropies (χ'), and factors α of the side-chain – side-chain potentials. See eqs. (6-8) of ref. 11 for the pertinent equations.

	FF1/FF2/OPT-W/OPT-WTF				OPT-WTFSA-1				OPT-WTFSA-2				OPT-ALL			
	$\sigma^{\perp}$	$\sigma^{\parallel}$	χ'	α	$\sigma^{\perp}$	$\sigma^{\parallel}$	χ'	α	$\sigma^{\perp}$	$\sigma^{\parallel}$	χ'	α	$\sigma^{\perp}$	$\sigma^{\parallel}$	χ'	α
Cys	2.67481	4.92722	-0.06957	0.01037	2.67481	4.92722	-0.06957	0.01037	2.67481	4.92722	-0.06957	0.01037	2.67481	4.92722	-0.06957	0.01037
Met	2.73388	5.10543	0.02632	0.06114	2.69990	5.50349	0.19370	0.06114	2.66569	5.74619	0.21948	0.06114	2.73807	4.97071	0.13242	0.06114
Phe	2.96646	4.20735	-0.03168	0.04483	2.96907	4.14576	0.02409	0.04483	2.95167	4.19875	0.04306	0.04483	2.98022	4.12295	0.05593	0.04483
Ile	2.88196	4.85140	0.01299	0.03928	2.89343	4.78508	0.01343	0.03928	2.89191	4.77862	0.06492	0.03928	2.90042	4.82548	0.03685	0.03928
Leu	3.02107	2.78489	0.04009	0.08542	3.02597	2.76857	0.01680	0.08542	3.01438	2.76742	-0.03516	0.08542	3.00663	2.74988	-0.04776	0.08542
Val	2.84143	3.58299	0.02644	0.03989	2.86281	3.57845	-0.04541	0.03989	2.86562	3.52710	-0.06473	0.03989	2.79924	3.70738	0.04469	0.03989
Trp	2.47734	7.86602	-0.11803	0.02495	2.52651	7.37799	-0.02817	0.02495	2.53643	7.26292	0.02282	0.02495	2.53077	7.36312	-0.07958	0.02495
Tyr	2.46119	7.42992	-0.05322	0.02324	2.42469	7.38422	-0.15664	0.02324	2.43595	7.27864	-0.23158	0.02324	2.39743	7.67080	-0.01624	0.02324
Ala	2.46532	1.96259	0.00199	0.08614	2.46807	2.01324	0.02983	0.08614	2.44371	2.07479	0.05011	0.08614	2.47895	2.00372	-0.02434	0.08614
Gly	2.49251	0.79878	0.10824	-0.07548	2.39766	0.79878	0.10824	-0.07548	2.40024	0.79878	0.10824	-0.07548	2.49330	0.79878	0.10824	-0.07548
Thr	2.57348	4.05809	-0.05637	-0.02661	2.57488	4.09886	-0.08637	-0.02661	2.58430	4.12794	-0.04805	-0.02661	2.58723	3.99776	0.00786	-0.02661
Ser	2.45640	1.88890	-0.04308	-0.01634	2.40900	2.23531	0.31441	-0.01634	2.42123	2.29761	0.48943	-0.01634	2.49952	1.52480	-0.41867	-0.01634
Gln	2.48478	3.19872	0.23541	0.05722	2.43051	3.22848	0.01989	0.05722	2.40663	3.28369	-0.07794	0.05722	2.42007	3.17826	0.07745	0.05722
Asn	2.48893	3.26733	0.17749	-0.04686	2.44940	3.30417	0.23433	-0.04686	2.43437	3.43903	0.34963	-0.04686	2.44010	3.61746	0.26441	-0.04686
Glu	2.50895	2.68481	0.34423	0.01510	2.49884	2.49514	0.14001	0.01510	2.51587	2.34401	0.09630	0.01510	2.51728	2.43095	0.06395	0.01510
Asp	2.50833	2.00430	0.17354	0.00850	2.49958	2.15945	0.26425	0.00850	2.52790	2.05434	0.19029	0.00850	2.48111	2.21237	0.41519	0.00850
His	2.42206	6.24463	-0.00333	0.02789	2.37755	6.27003	-0.13500	0.02789	2.39070	6.16602	-0.10227	0.02789	2.40569	6.40784	0.29442	0.02789
Arg	2.27146	8.19595	0.17762	0.00769	2.32781	7.37373	-0.04939	0.00769	2.33339	7.23737	-0.11014	0.00769	2.29047	7.99586	0.13028	0.00769
Lys	2.45207	13.47483	0.92981	0.10335	2.40613	14.03118	0.92726	0.10335	2.41915	13.70834	0.92452	0.10335	2.45675	13.51144	0.92726	0.10335
Pro	2.70261	2.66324	-0.12435	-0.00983	2.70311	2.68607	-0.06605	-0.00983	2.68663	2.72650	-0.02977	-0.00983	2.70693	2.63940	-0.14172	-0.00983

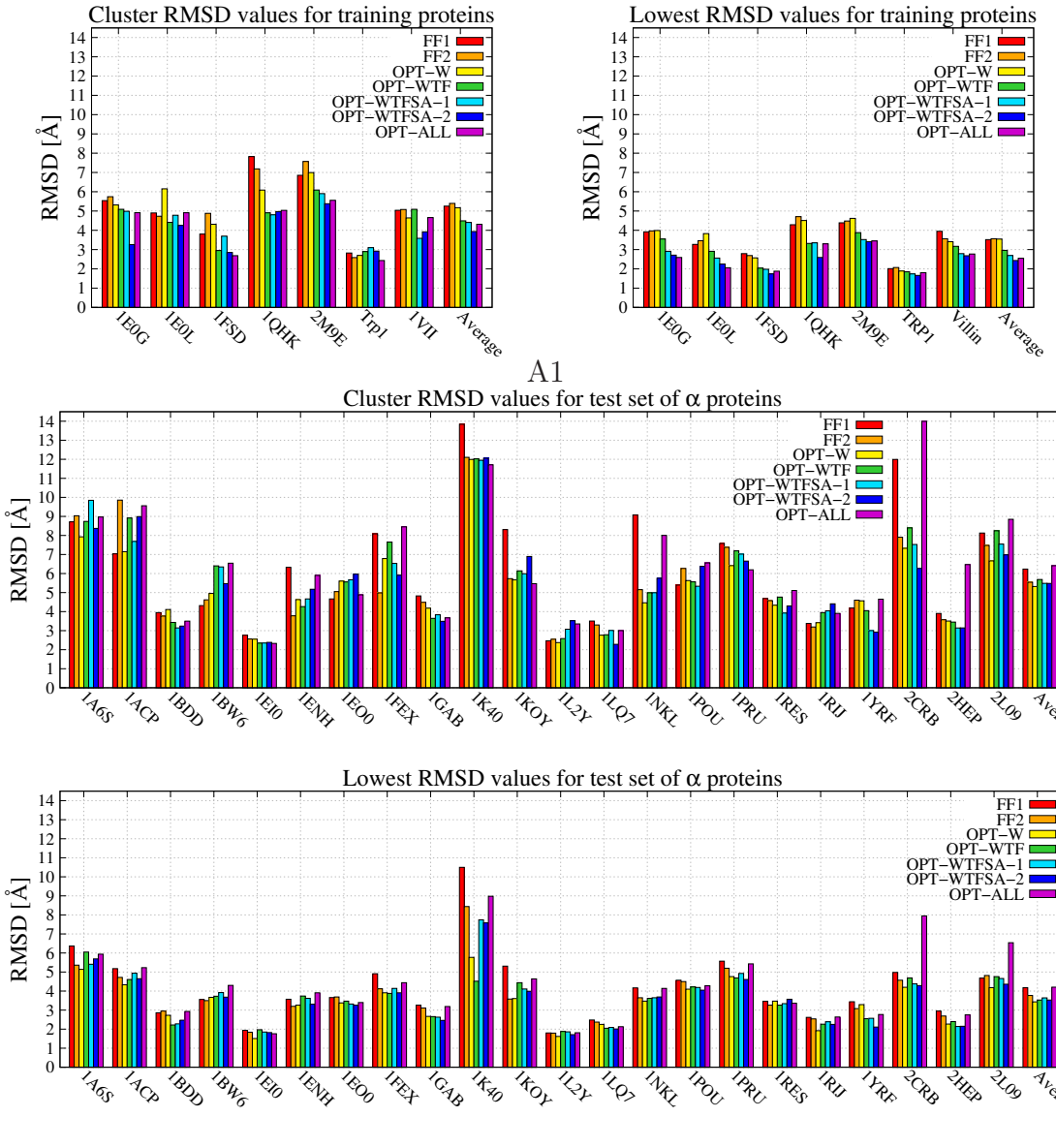
Table S4: Original (upper triangle, pertaining to the FF1, FF2, OPT-W, OPT-WTF, OPT-WTFSA-1, and OPT-WTFSA-2 variants of the UNRES force field) and optimized (lower triangle, pertaining to the OPT-ALL variant of the UNRES force field) well-depths (ϵ°) of the Gay-Berne potentials of the side chain – side chain interactions. See eq. (6) of ref. 11.

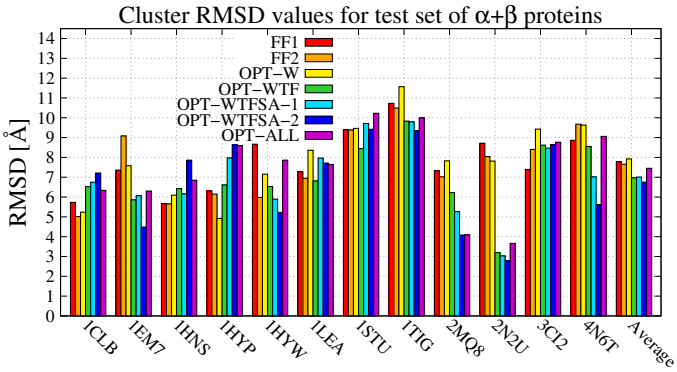
	Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala	Gly	Thr	Ser	Gln	Asn	Glu	Asp	His	Arg	Lys	Pro	
	5.6054	6.2200	6.2160	6.4387	6.2098	5.9596	5.4310	4.8790	5.2638	5.4962	4.2928	4.3582	4.2668	3.6814	3.5405	3.7027	4.7178	3.3812	3.7936	4.5157	Cys
		6.6297	6.6717	6.8169	6.8379	6.3512	6.1425	5.5200	5.4859	4.9383	4.2795	4.0535	4.2086	3.5388	3.4210	2.7996	4.8164	3.8791	3.5878	4.6457	Met
Cys	5.6054		6.6424	6.9716	6.9241	6.5291	6.1395	5.4416	5.2914	4.7882	4.1302	3.9405	3.9023	3.6079	3.0810	3.0183	4.7936	3.8712	3.6826	4.4873	Phe
Met	6.2200	6.6297		7.3272	7.2970	7.0495	6.2566	5.8134	5.8845	5.3464	4.7147	4.4865	4.3092	3.6928	4.0101	3.6585	4.5902	4.4682	4.6334	4.9024	Ile
Phe	6.2160	3.5430	5.1941		7.0106	6.8342	6.2048	5.5802	5.6717	5.2011	4.1967	4.2384	3.8954	3.5679	3.1136	2.7623	4.5092	4.0238	3.9800	4.8087	Leu
Ile	6.4387	7.0446	5.2348	6.0791		6.5354	5.8844	5.1101	5.5515	4.9588	4.2031	4.0352	3.6506	3.4640	3.1611	2.7976	4.0423	3.4416	3.8621	4.5934	Val
Leu	6.2098	4.9614	5.5283	6.7613	4.8392		5.2829	4.8298	4.7575	4.7250	3.5656	3.5613	3.9273	3.7665	3.5862	3.5523	4.6509	4.2424	4.0988	4.5080	Trp
Val	5.9596	5.4874	5.0196	8.5032	5.3041	6.0107		4.2223	4.1627	3.9786	3.1623	2.9380	3.1366	2.8026	2.6576	2.8733	3.8786	3.4443	3.4405	4.0915	Tyr
Trp	5.4310	1.0102	5.5233	-0.0005	2.2465	3.0294	5.0463		4.3861	3.6520	3.0265	2.5681	2.5002	2.1393	1.4707	1.7373	3.1045	2.0152	1.8196	3.6396	Ala
Tyr	4.8790	1.4072	3.9744	4.1498	5.0580	5.6216	4.2918	4.2896		2.5017	2.7880	2.1425	1.0742	1.3236	-0.2712	0.7613	2.8627	1.5002	-0.2393	3.5381	Gly
Ala	5.2638	5.1972	4.1732	5.1544	3.7444	5.1109	3.4040	2.2234	3.2841		2.2904	2.2467	1.5054	1.4032	0.9676	1.3076	2.8595	1.9833	-0.0086	2.9558	Thr
Gly	5.4962	3.4340	4.1256	4.4096	2.8450	7.1205	4.1228	2.6728	1.6056	1.4018		1.2800	0.7690	0.9120	-0.0744	0.3670	2.4289	1.4975	-0.2134	2.9415	Ser
Thr	4.2928	9.9519	4.2443	2.2958	2.9477	1.8481	4.3772	3.7117	3.0989	0.9355	1.4194		-0.6792	0.4532	-0.7590	-0.3617	1.6803	0.6775	-0.5355	2.6209	Gln
Ser	4.3582	2.4482	2.8897	3.0660	0.7581	1.1833	-0.0435	2.4586	1.5265	0.4631	-0.1897	2.9420		0.4136	-0.1637	0.2213	2.1287	0.3896	-0.2354	2.3255	Asn
Gln	4.2668	-0.7489	3.6797	-2.1162	2.8771	5.1260	3.6335	3.4384	2.3779	1.6402	-0.0341	4.9137	-0.0362		-3.5194	-2.0157	1.8356	2.7489	2.0098	1.7976	Glu
Asn	3.6814	1.7462	2.7657	0.5993	1.6790	5.3978	5.7682	1.4773	5.4685	4.5665	0.6740	0.9284	0.3014	1.0013		-1.3533	2.5504	2.8203	1.6254	1.8625	Asp
Glu	3.5405	4.0445	1.8734	1.0084	2.7985	2.3438	2.8688	2.4138	-0.3033	-0.1846	0.1992	-0.2032	0.0001	-0.0638	-7.5304		3.7293	2.2944	-0.0304	3.1116	His
Asp	3.7027	1.1786	3.8900	2.1315	2.9246	5.9179	2.9626	2.4224	2.1939	0.2680	1.3195	0.2542	1.2893	0.0426	-1.8411	-0.7717		-0.0827	-1.6043	2.4440	Arg
His	4.7178	-9.9996	6.2315	5.3012	8.0419	10.0000	7.9140	-0.7114	5.1575	0.4657	-0.4737	-1.6276	-6.7068	1.0383	3.6001	9.9997	3.7293		-4.3898	2.3665	Lys
Arg	3.3812	2.5607	4.2737	3.8328	2.7537	1.9972	3.3338	4.1555	0.3010	1.5032	2.7245	-0.0737	4.0935	0.1571	1.7124	4.7385	8.8242	-0.0696		4.1928	Pro
Lys	3.7936	5.0345	3.9630	2.0472	3.3606	4.0340	3.0336	2.3499	1.3946	-0.2147	-0.0049	-0.0107	-0.2746	-0.1576	1.4580	1.6274	-0.2451	-1.3278	-3.1313		
PRO	4.5157	4.3415	1.5645	5.2892	3.4390	3.9049	4.2755	4.0658	1.0697	1.8963	-0.7864	0.0000	1.0359	2.6648	2.8905	-0.1232	-9.9997	2.9767	1.3032	3.3529	

Table S5: The ranks (#) of the most native-like clusters and fractions of the conformations of these clusters (frac) in the conformational ensembles 10 K below the calculated folding-transition temperature.

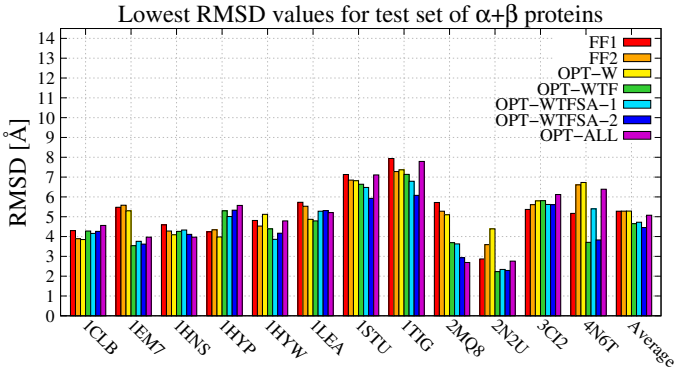
	FF1		FF2		OPT-W		OPT-WTF		OPT-WTFSA-1		OPT-WTFSA-2		OPT-ALL	
α-proteins	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac
1A6S	1	0.40918	4	0.10702	3	0.21596	5	0.11559	3	0.20143	4	0.14142	3	0.20576
1ACP	2	0.32233	3	0.15585	4	0.16817	1	0.33381	1	0.30821	4	0.10814	1	0.29318
1BDD	2	0.24853	1	0.29848	3	0.18359	4	0.15495	2	0.22900	3	0.19888	1	0.29965
1BW6	2	0.23786	4	0.11602	2	0.21591	5	0.08180	4	0.17214	3	0.18469	2	0.28281
1EI0	1	0.55121	4	0.22884	1	0.37166	3	0.21807	3	0.14955	1	0.34535	1	0.35038
1ENH	2	0.23989	2	0.23781	1	0.33850	3	0.20712	3	0.20142	2	0.20916	4	0.15751
1EO0	3	0.16130	3	0.15265	4	0.17195	2	0.27406	5	0.11288	4	0.19223	5	0.08081
1FEX	2	0.24580	3	0.18348	4	0.16037	2	0.25643	5	0.15156	4	0.14900	1	0.36761
1GAB	5	0.10753	2	0.21201	4	0.15629	4	0.12109	3	0.22257	3	0.16571	5	0.08940
1K40	1	0.62545	1	0.61787	1	0.43087	2	0.21669	4	0.13692	1	0.43538	5	0.17763
1KOY	2	0.20771	2	0.23459	4	0.13243	5	0.15736	5	0.16486	3	0.23214	2	0.23087
1L2Y	1	0.32136	1	0.35007	1	0.26890	1	0.30658	2	0.28090	1	0.32426	2	0.27485
1LQ7	2	0.25181	2	0.31201	2	0.28937	5	0.04485	4	0.15839	1	0.46446	1	0.53711
1NKL	1	0.32305	4	0.19045	5	0.10593	1	0.29489	2	0.29388	1	0.32508	1	0.26312
1POU	3	0.13298	5	0.10951	1	0.29912	3	0.21792	2	0.19293	5	0.15057	4	0.17665
1PRU	1	0.31193	5	0.12318	4	0.15271	1	0.28605	3	0.19973	2	0.27957	4	0.17295
1RES	2	0.25745	3	0.17112	5	0.08126	2	0.32649	3	0.18995	2	0.21522	4	0.18432
1RIJ	4	0.06171	4	0.04223	3	0.22940	1	0.28597	1	0.30009	1	0.35481	1	0.40367
1YRF	5	0.12524	1	0.48825	2	0.23210	3	0.16443	3	0.18196	4	0.13556	3	0.19285
2CRB	5	0.08456	2	0.25035	1	0.34330	3	0.18369	3	0.21175	4	0.06783	1	0.36535
2HEP	1	0.31325	1	0.40163	3	0.22276	1	0.32546	1	0.47587	4	0.12374	4	0.15389
2L09	3	0.17451	1	0.27128	2	0.22380	1	0.28589	1	0.34325	1	0.21918	1	0.25810
α-β-proteins	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac
1CLB	2	0.23730	5	0.09608	5	0.09910	4	0.19374	4	0.14907	4	0.18143	3	0.16180
1EM7	2	0.22920	3	0.14638	2	0.22306	5	0.06588	5	0.02448	4	0.07216	4	0.11807
1HNS	4	0.10141	4	0.10447	2	0.28175	2	0.24052	4	0.16307	2	0.20955	3	0.20627
1HYP	2	0.22789	5	0.11865	1	0.40150	3	0.08478	2	0.20136	2	0.23522	1	0.26843
1HYW	2	0.23761	4	0.15182	4	0.10060	5	0.11364	4	0.15359	5	0.06472	5	0.14039
1LEA	1	0.40141	4	0.14611	4	0.11665	1	0.30447	3	0.20291	5	0.16338	5	0.11191
1STU	3	0.17981	3	0.14049	4	0.13160	5	0.15049	2	0.21611	2	0.28067	5	0.13141
1TIG	1	0.34037	3	0.10754	3	0.18910	5	0.07307	4	0.16779	1	0.43674	5	0.06141
2MQ8	1	0.34734	1	0.27475	1	0.27514	1	0.25755	2	0.36046	3	0.20457	1	0.45887
2N2U	1	0.39779	5	0.09894	1	0.23848	1	0.37609	1	0.31071	1	0.34026	4	0.14874
3CI2	5	0.06479	3	0.20255	5	0.10631	2	0.24750	2	0.28305	2	0.28242	5	0.11766
4N6T	1	0.27144	4	0.15932	4	0.18200	2	0.22505	4	0.10289	4	0.08948	5	0.13584
β-proteins	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac	#	frac
1BK2	3	0.16002	4	0.11109	3	0.17096	2	0.30956	3	0.16443	3	0.17596	5	0.11187
1ED7	4	0.19982	1	0.30755	5	0.06110	5	0.11772	1	0.34444	2	0.21861	2	0.29331
1GH5	4	0.14201	2	0.20212	5	0.10735	4	0.18355	4	0.12696	3	0.11753	3	0.18607
1LE1	4	0.12377	4	0.06201	5	0.07622	5	0.09289	1	0.30374	1	0.49052	1	0.31042
1WIU	2	0.22637	5	0.16585	3	0.19982	2	0.20061	3	0.18286	1	0.45517	2	0.25141
2JNI	2	0.25868	1	0.21932	2	0.21897	1	0.24802	3	0.15109	2	0.23118	5	0.13372
2KYW	2	0.23052	5	0.06799	3	0.16781	2	0.20130	3	0.18506	3	0.15128	4	0.11027
2LGN	5	0.10798	4	0.11627	2	0.23659	3	0.19113	5	0.09794	3	0.18039	3	0.17194
2LVC	5	0.06958	5	0.05152	3	0.22790	1	0.48060	5	0.06217	4	0.07875	2	0.21182
2LXZ	1	0.24703	4	0.15169	3	0.17633	5	0.06588	5	0.05993	5	0.09111	4	0.12357
3PUC	4	0.12826	4	0.09811	1	0.28613	4	0.12290	3	0.13116	3	0.14472	1	0.37178
4QRL	5	0.09040	2	0.18155	5	0.10146	2	0.24740	2	0.20617	3	0.13052	3	0.25969

Figure S1: Averaged over native-like clusters and minimal over the whole MREMD simulations C^{α}-RMSD (panels A1 – D2), TM-score (panels E – H) , and GDT_TS (panels I – L) values of the training (panels A1, A2, E, I) and test (panels B1 – D2, F – H, J – L) proteins.

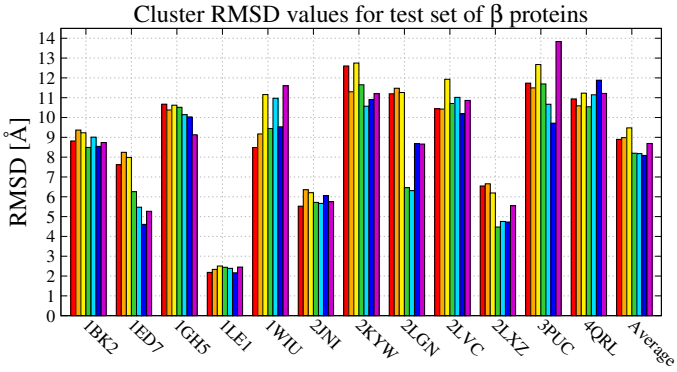




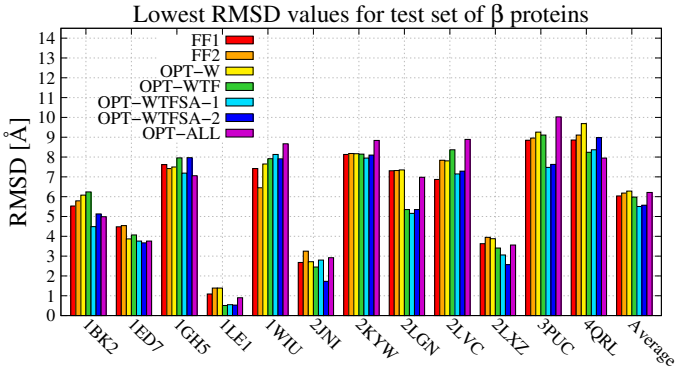
C1



C2

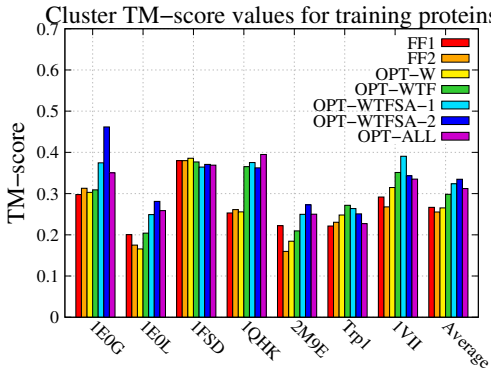


D1

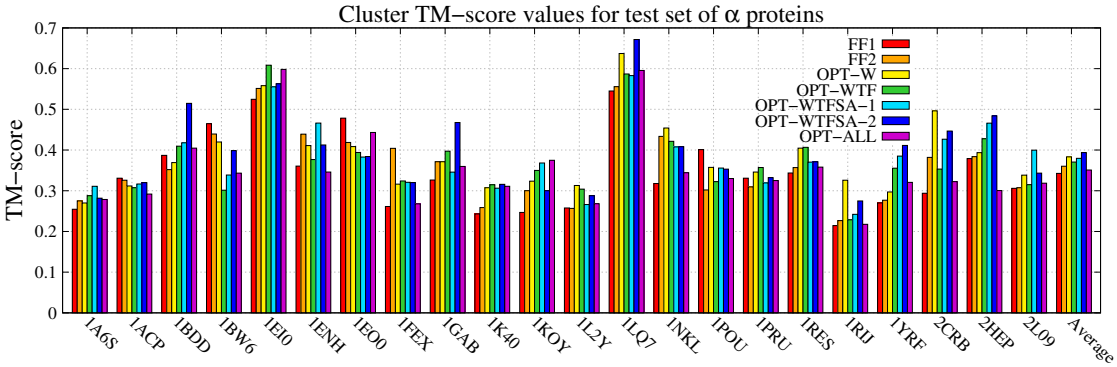


D2

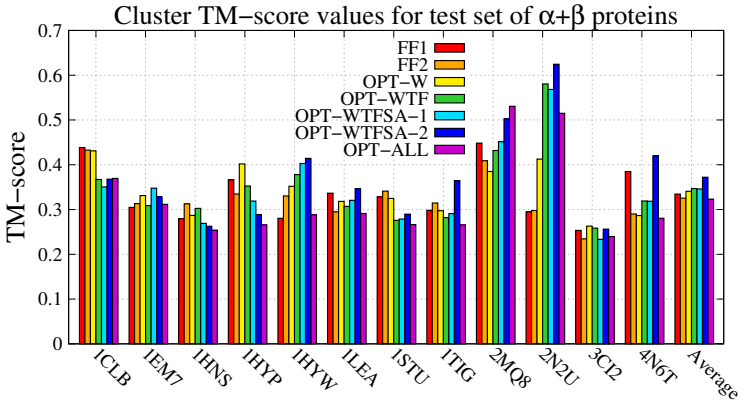
Figure S1 (continued)



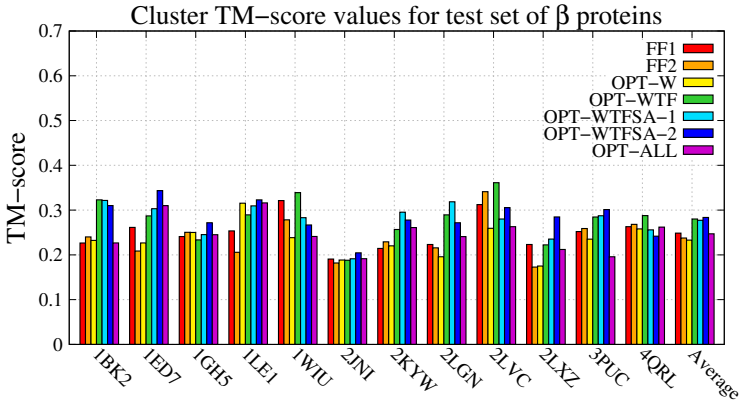
E



F

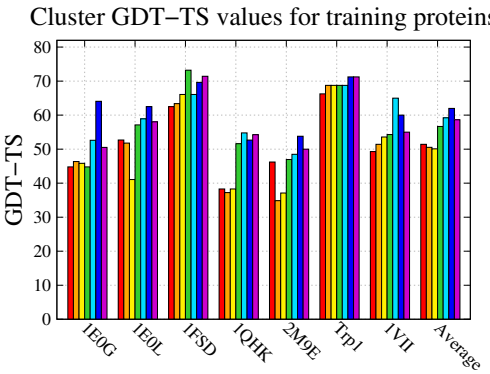


G

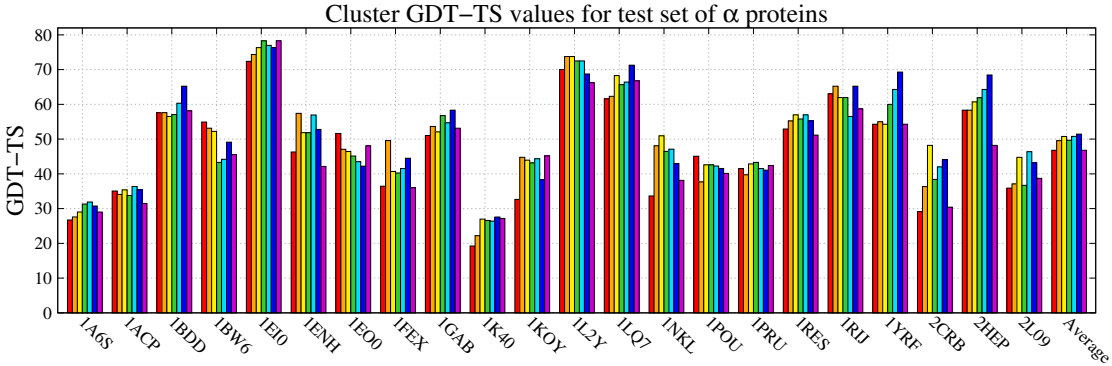


H

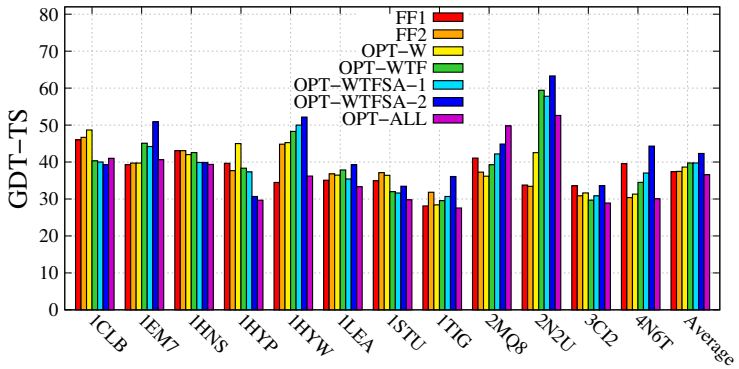
Figure S1 (continued)



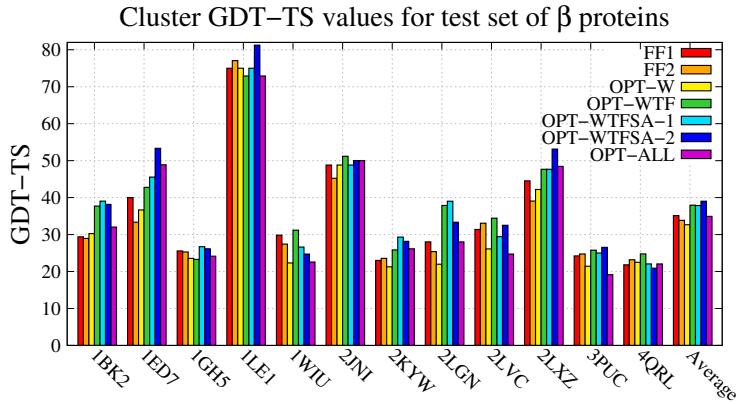
I



J



K



L

Figure S1 (continued)