

Supporting Information for: Force Field-Induced Bias in the Structure of A β ₂₁₋₃₀: A Comparison of OPLS, AMBER, CHARMM, and GROMOS Force-Fields

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Organization and layout of this section.

This section contains tables and figures that supplement the computational methods and conclusions contained in the main text. These tables and figures are discussed in and are directly referenced from the main text. For this reason, they are only presented below with respective table and figure captions, but without further discussion.

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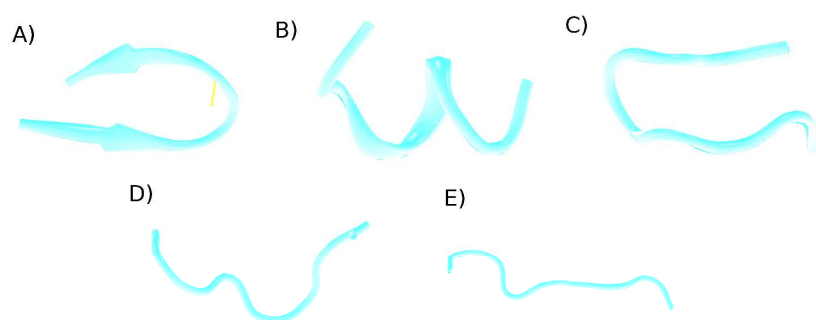


Figure S1) Sample representations of secondary structures. A) β , B) Helix, C) Bridge, D) Turn, E) Coil

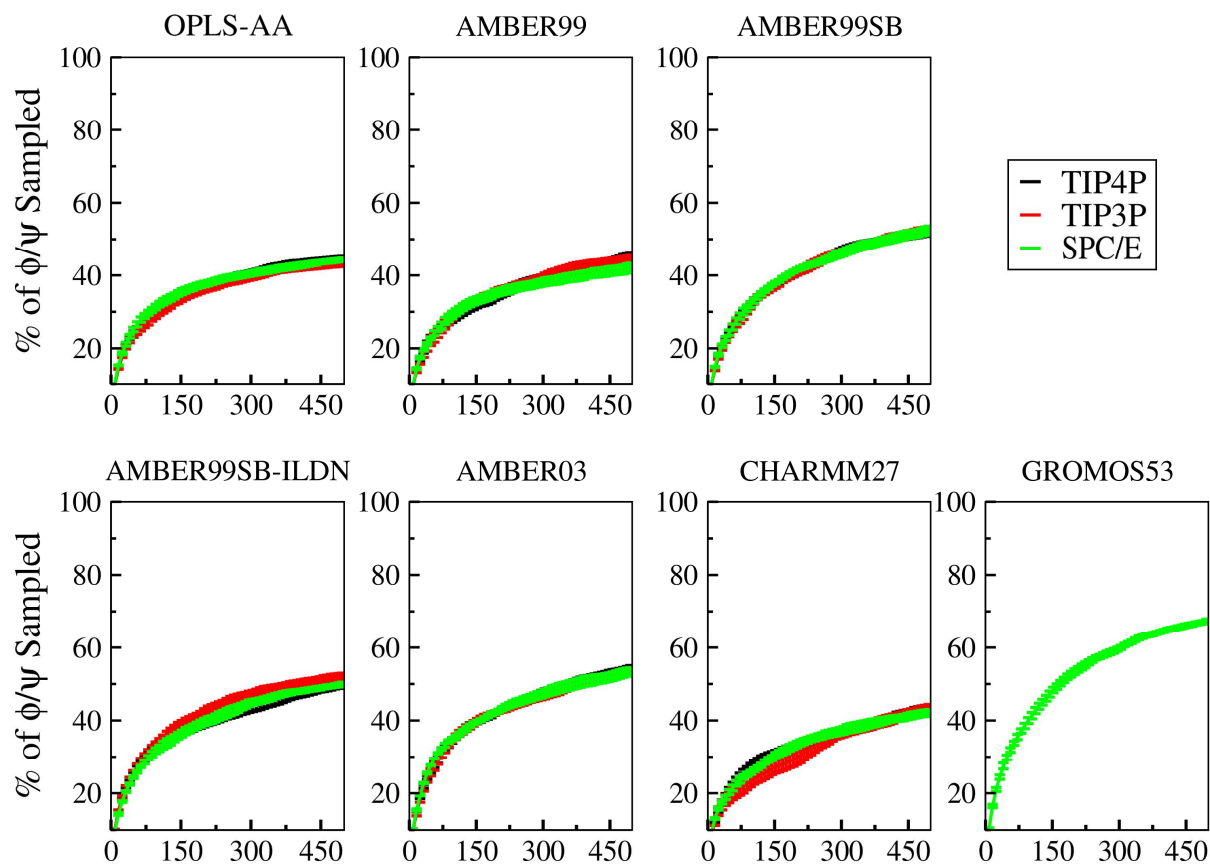


Figure S2. Average percentage of Ramachandran space sampled as a function of simulation time. Error bars are standard error of the mean. As simulation approaches convergence, the percentage of Ramachandran space sampled approaches an asymptote.

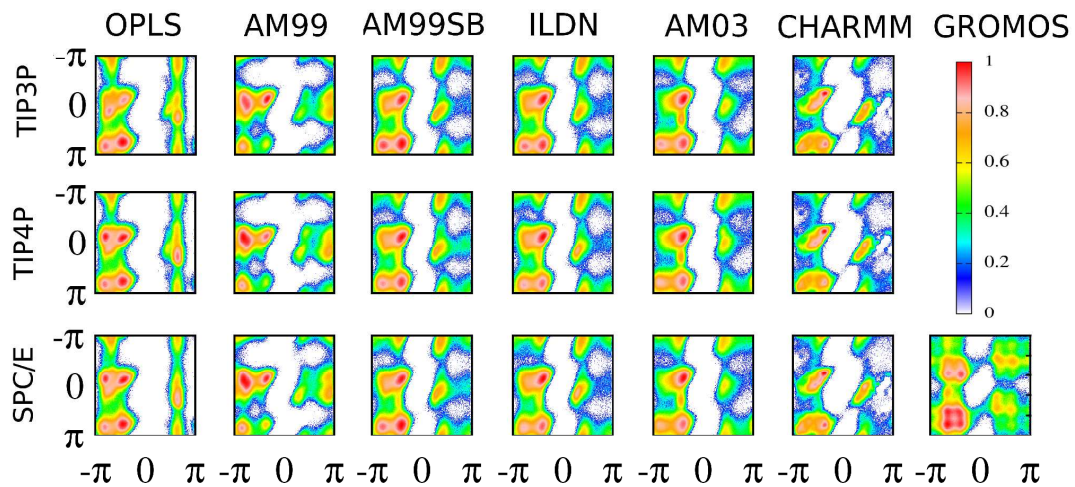


Figure S3) Composite (all frames from all trajectories of noted force-field/water model choice) Ramachandran Spaces.

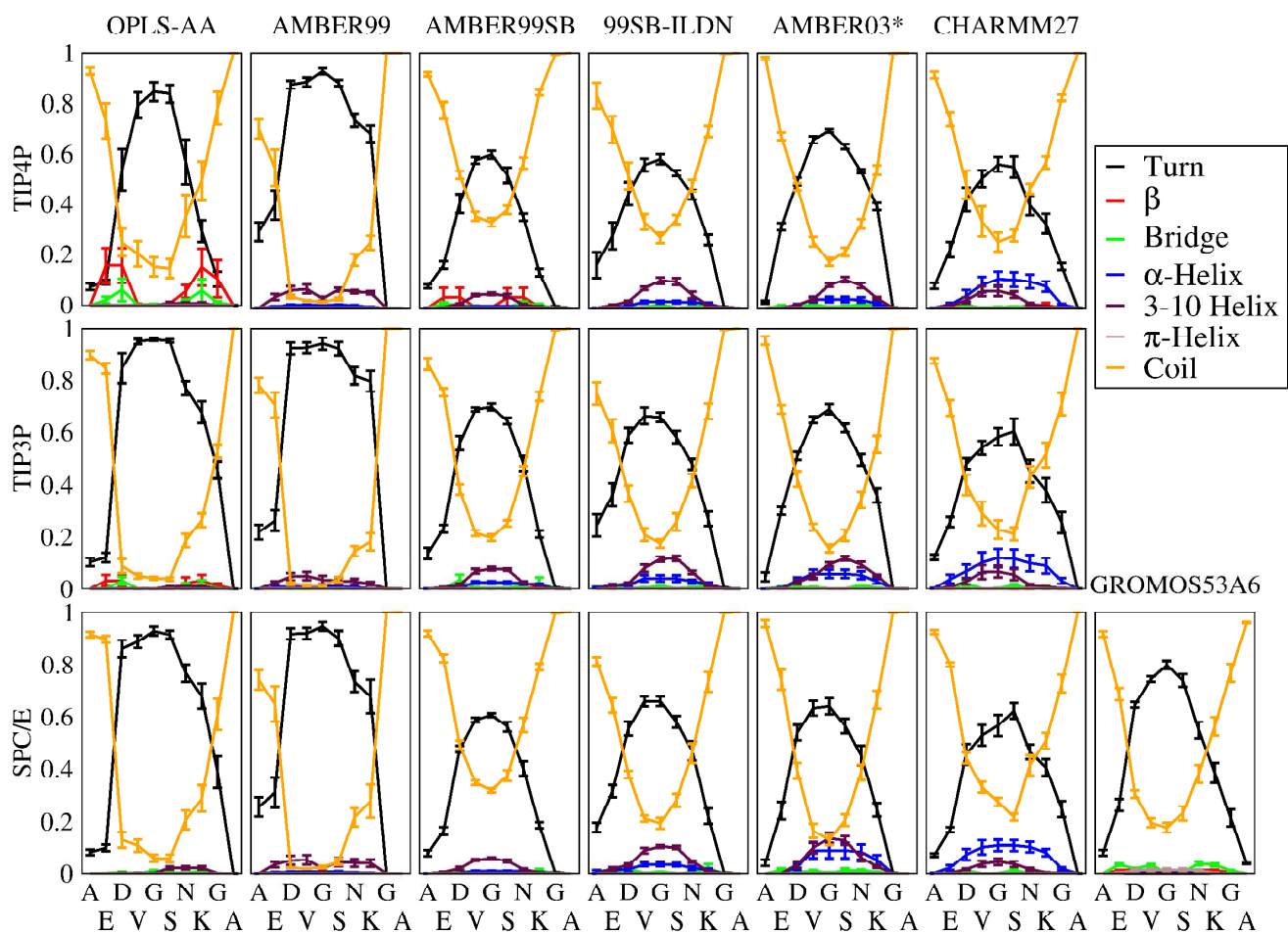


Figure S4. Average secondary structure propensities per amino acid. Error bars are standard error of the mean.

OPLS-AA					AMBER 99SB-ILDN			
Name		Description	Sigma	Epsilon	Name	Description	Sigma	Epsilon
opls_235	C	C=O in amide	3.75000e-01	4.39320e-01	C	Carbon in carbonyl group	3.9967e-01	3.59824e-01
opls_135	CT	Alkane carbon	3.50000e-01	2.76144e-01	CT	Aliphatic carbon	3.9967e-01	4.57730e-01
opls_240	H	H on N in primary amide	0.00000e+00	0.00000e+00	H	Hydrogen bonded to nitrogen atoms	1.06908e-01	6.56888e-02
opls_140	HC	Alkane hydrogen	2.50000e-01	1.25520e-01	HC	Aliphatic hydrogen bonded to carbon	2.64953e-01	6.56888e-02
opls_155	HO	Hydrogen in mono alcohols	0.00000e+00	0.00000e+00	HO	Hydrogen in hydroxyl group	0.00000e+00	0.00000e+00
opls_236	O	C=O in amide	2.96000e-01	8.78640e-01	O	Oxygen in carbonyl group	2.95992e-01	8.78640e-01
opls_272	O2	O in COO-carboxylate, peptide terminus	2.96E-001	8.78640E-01	O2	Oxygen in carboxyl and phosphate groups	2.95992e-01	8.78640E-01
opls_154	OH	Oxygen in mono alcohols	3.12000e-01	7.11280e-01	OH	Oxygen in hydroxyl group	3.06647e-01	8.80314e-01
opls_790	OW	Oxygen in TIP4P Water	3.21500e-01	5.85760e-01	OW_tip4p	Oxygen in TIP4P Water	3.15365e-01	6.48520e-01

Table S1. Table that lists the OPLS-AA parameters with their original values (on the lhs) that were replaced with the AMBER99SB-ILDN parameters (on the rhs). This modified OPLS-AA force field was used to investigate the origin of the differences found between these two force fields in the structural properties of the decapeptide.

Table S2. Results on the secondary structure found using the modified OPLS-AA force field with the AMBER99SB-ILDN non-bonded parameters. Due to rounding error, some of the percentages may not add to 100%.

	Average Percentages (%) for the five trajectories	Standard Error of the Mean
Turn	51.2	5.8
Beta	0.2	0.1
Coil	1.7	0.5
Helix	46.8	6.1

Table S3. Results on the secondary structure found using the modified AMBER99SB-ILDN force field with the OPLS-AA non-bonded parameters. Due to rounding error, some of the percentages may not add to 100%.

	Average Percentages (%) for the ten trajectories	Standard Error of the Mean
Turn	57.9	1.6
Beta/Bridge	4.96	3
Coil	34.3	2.3
Helix	13.3	1.7

Cystine Dimer water-vacu energy comparisons:

Methodology: Two dimers of Cystine (two sets of Cystine dimers) separated by ~0.35nm were simulated for 5ns in the NPT (~1atm, 303K) ensemble with restraints to hold the center of mass distance between the two dimers roughly constant. This was performed for each force-field with the cystine dimers solvated in TIP3P water (except GROMOS where SPC/E was used) and *in vacu*. The same bond constraints used in the main text are also used here, along with a 2fs integration timestep. Absolute relative differences (unit-less ratio of changes to the energies) to the short-range lennard-jones and electrostatic interactions between the Cystine dimers from switching from *in vacu* conditions to aqueous conditions are reported in table S4 below.

Force-field	LJ (SR)	Electrostatic (SR)
OPLS-AA	0.444 (0.095)	0.156 (0.0709)
AMBER99	1.547 (0.033)	8.783 (0.208)
AMBER99SB	1.641 (0.0566)	1.533 (0.703)
AMBER99SBILDN	1.629 (0.050)	1.371 (0.492)
AMBER03	1.467 (0.152)	0.824 (0.52)
CHARMM22/27-CMAP	0.321 (0.117)	0.323 (0.056)
GROMOS53A6	0.5198 (0.048)	0.749 (0.0323)

Table S4) Absolute relative differences of non-bonded terms of two cystine dimers. Comparison is made between *in vacu* and aqueous solution (changes are relative to vacuum energies). Standard deviations are reported in parenthesis.