Supporting Information A. Using MP2/cc-pVTZ//B3LYP/6-31G results as the "true" value.**

Table S1. The mainchain and sidechain dihedral angles in the five selected conformations for 20 amino acids.

		ϕ	ψ	χ_1	χ_2	χ_3	χ_4
Pro[a]	α_R	-57.0	-47.0	-26.1	37.8	-34.6	19.1
	α_L	57.0	47.0	-15.0	32.3	-37.0	29.1
	β	-119.0	113.0	4.5	18.0	-33.8	38.2
	βa	-140.0	135.0	37.5	-23.3	0.6	24.0
	PPII	-79.0	150.0	-19.4	33.9	-35.4	24.5
Gly	α_R	-57.0	-47.0				
	α_L	57.0	47.0				
	β	-119.0	113.0				
	βa	-140.0	135.0				
	PPII	-79.0	150.0				
Ala	α_R	-57.0	-47.0				
	α_L	57.0	47.0				
	β	-119.0	113.0				
	βa	-140.0	135.0				
	PPII	-79.0	150.0				
Val	α_R	-57.0	-47.0	171.9			
	α_L	57.0	47.0	-171.2			
	β	-119.0	113.0	178.9			
	βa	-140.0	135.0	178.4			
	PPII	-79.0	150.0	173.5			
Leu	α_R	-57.0	-47.0	179.3	61.7		
	α_L	57.0	47.0	-61.4	178.5		
	β	-119.0	113.0	178.2	61.8		
	βa	-140.0	135.0	-65.8	171.3		
	PPII	-79.0	150.0	-62.5	175.9		
Ile	α_R	-57.0	-47.0	-67.5	168.7		
	α_L	57.0	47.0	-51.5	-174.3		
	β	-119.0	113.0	-59.6	172.6		
	βa	-140.0	135.0	-61.0	172.5		
	PPII	-79.0	150.0	62.2	171.1		
Met	α_R	-57.0	-47.0	-69.3	175.4	68.5	
	α_L	57.0	47.0	-61.1	-58.9	-65.8	
	β	-119.0	113.0	-178.1	179.6	-75.1	
	βa	-140.0	135.0	178.7	174.7	72.0	
	PPII	-79.0	150.0	-62.6	-62.4	-68.9	
Phe	α_R	-57.0	-47.0	178.3	79.3		
	α_L	57.0	47.0	-58.3	105.0		
	β	-119.0	113.0	-63.1	90.2		
	βa	-140.0	135.0	-61.3	92.8		
	PPII	-79.0	150.0	-72.5	99.7		

[a] χ_3 and χ_4 for proline were obtained from the geometry optimization at B3LYP/6-31G**.

Tyr	α_R	-57.0	-47.0	178.3	79.6		
	α_L	57.0	47.0	-58.4	104.9		
	β	-119.0	113.0	-62.0	91.2		
	βa	-140.0	135.0	-60.6	90.6		
	PPII	-79.0	150.0	-71.6	98.3		
His	α_R	-57.0	-47.0	177.6	74.2		
	α_L	57.0	47.0	-57.2	-62.4		
	β	-119.0	113.0	-59.8	-81.0		
	βa	-140.0	135.0	-61.8	-81.6		
	PPII	-79.0	150.0	-67.2	-79.8		
Trp	α_R	-57.0	-47.0	-179.4	85.4		
	α_L	57.0	47.0	-57.2	104.8		
	β	-119.0	113.0	-176.4	10.5		
	βa	-140.0	135.0	-63.7	89.7		
	PPII	-79.0	150.0	-67.9	99.7		
Cys	α_R	-57.0	-47.0	-69.2			
	α_L	57.0	47.0	-62.2			
	β	-119.0	113.0	-178.5			
	βa	-140.0	135.0	-179.8			
	PPII	-79.0	150.0	-63.5			
Ser	α_R	-57.0	-47.0	-66.5			
	α_L	57.0	47.0	-61.2			
	β	-119.0	113.0	177.4			
	βa	-140.0	135.0	179.7			
	PPII	-79.0	150.0	66.9			
Thr	α_R	-57.0	-47.0	-61.7			
	α_L	57.0	47.0	60.5			
	β	-119.0	113.0	-59.9			
	βa	-140.0	135.0	-58.7			
	PPII	-79.0	150.0	61.5			
Asn	α_R	-57.0	-47.0	-72.8	-19.4		
	α_L	57.0	47.0	-163.8	26.7		
	β	-119.0	113.0	-175.7	-23.2		
	βa	-140.0	135.0	-61.8	-77.4		
	PPII	-79.0	150.0	-70.3	-22.8		
Gln	α_R	-57.0	-47.0	-70.6	174.5	-4.3	
	α_L	57.0	47.0	-64.8	-69.0	-51.0	
	β	-119.0	113.0	-178.7	180.0	5.8	
	βa	-140.0	135.0	-177.5	178.4	-4.4	
	PPII	-79.0	150.0	-61.1	-62.7	-54.3	
Asp	α_R	-57.0	-47.0	-72.4	-12.6		
	α_L	57.0	47.0	-162.6	16.3		
	β	-119.0	113.0	-177.6	-5.9		
	βa	-140.0	135.0	-68.3	-69.1		
	PPII	-79.0	150.0	-71.6	-12.3		

Glu	α_R	-57.0	-47.0	-178.1	178.6	-0.7	
	α_L	57.0	47.0	-62.0	179.9	3.3	
	β	-119.0	113.0	-177.0	179.0	3.8	
	βa	-140.0	135.0	-62.6	-178.4	-1.3	
	PPII	-79.0	150.0	-64.5	-178.2	-2.7	
Lys	α_R	-57.0	-47.0	-178.3	177.1	178.0	-179.0
	α_L	57.0	47.0	-63.8	-179.4	-178.6	175.5
	β	-119.0	113.0	-63.7	-178.4	178.5	-174.7
	βa	-140.0	135.0	-67.0	-176.3	179.9	178.8
	PPII	-79.0	150.0	-67.4	-179.2	179.3	179.4
Arg	α_R	-57.0	-47.0	-70.6	178.1	-177.9	177.1
	α_L	57.0	47.0	-59.2	178.2	72.0	83.2
	β	-119.0	113.0	-72.2	175.7	-174.8	-82.8
	βa	-140.0	135.0	-62.6	-70.2	-175.6	-87.0
	PPII	-79.0	150.0	-67.3	-177.5	178.0	-179.5

Table S2. Relative energies (with reference to the α_R conformation) calculated by the different methods for the five conformations of each tetrapeptide (kcal/mol).

MP2/cc-pVTZ//B3LYP/6-31G**						M05-2X/cc-pVTZ//M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	2.24	4.26	5.29	1.76	Pro	0.00	2.23	2.59	3.55	-0.42
Gly	0.00	1.55	3.67	1.74	2.85	Gly	0.00	1.16	1.97	-0.93	0.90
Ala	0.00	2.23	3.44	1.01	2.91	Ala	0.00	1.69	1.76	-0.90	0.77
Val	0.00	3.61	2.15	0.18	3.17	Val	0.00	3.15	0.71	-1.84	1.14
Leu	0.00	3.24	3.37	0.79	3.01	Leu	0.00	2.73	1.95	-1.18	1.21
Ile	0.00	4.15	1.97	0.13	2.27	Ile	0.00	3.62	0.57	-1.79	0.44
Met	0.00	-0.12	3.05	0.87	1.53	Met	0.00	-0.76	1.62	-0.82	-0.03
Phe	0.00	-0.62	0.55	-0.91	2.69	Phe	0.00	-1.93	-1.29	-3.27	0.23
Tyr	0.00	-0.43	0.37	-0.97	2.51	Tyr	0.00	-1.63	-1.94	-3.53	0.17
His	0.00	0.05	1.28	0.13	2.32	His	0.00	-1.17	-0.53	-1.89	0.11
Trp	0.00	-0.19	2.54	-0.27	2.40	Trp	0.00	-1.71	-0.12	-2.89	-0.28
Cys	0.00	0.95	1.78	1.15	4.06	Cys	0.00	0.21	2.36	-0.59	2.26
Ser	0.00	1.33	3.90	1.13	3.62	Ser	0.00	0.38	2.52	-0.89	1.93
Thr	0.00	1.99	5.44	4.22	4.00	Thr	0.00	1.45	4.14	2.52	2.48
Asn	0.00	-0.84	1.36	1.53	3.52	Asn	0.00	-1.70	-0.47	0.22	1.75
Gln	0.00	2.06	2.63	0.43	-1.74	Gln	0.00	2.12	1.07	-1.62	-3.22
Asp	0.00	16.70	-0.44	7.01	12.97	Asp	0.00	16.99	-1.12	6.41	12.20
Glu	0.00	5.34	-0.63	2.91	7.20	Glu	0.00	4.86	-0.87	0.85	5.73
Lys	0.00	2.92	3.51	0.42	0.78	Lys	0.00	2.41	2.06	-1.54	-1.36
Arg	0.00	-4.06	-1.33	-18.48	-4.90	Arg	0.00	-4.48	-2.91	-19.64	-7.46

M05-2X-D[a]/cc-pVTZ//M05-2X/6-31G**						M05-2X/6-31G**//M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	3.18	8.51	11.03	2.74	Pro	0.00	0.99	4.03	5.10	2.39
Gly	0.00	2.35	5.10	2.57	4.24	Gly	0.00	0.23	4.08	0.85	3.11
Ala	0.00	3.27	5.01	2.46	3.97	Ala	0.00	0.35	3.69	0.95	2.79
Val	0.00	6.04	3.28	1.19	4.43	Val	0.00	1.29	2.79	-0.16	2.93
Leu	0.00	4.72	4.59	1.67	4.14	Leu	0.00	1.36	4.22	0.52	3.52
Ile	0.00	6.94	3.01	1.25	2.47	Ile	0.00	1.73	2.69	0.08	2.20
Met	0.00	0.89	4.40	2.06	2.44	Met	0.00	-2.30	3.67	1.03	2.03
Phe	0.00	0.27	0.15	-1.68	3.52	Phe	0.00	-3.40	0.21	-1.74	2.49
Tyr	0.00	0.52	-0.61	-1.95	3.64	Tyr	0.00	-3.14	-0.54	-2.42	2.33
His	0.00	0.93	0.45	-0.21	3.22	His	0.00	-2.40	0.97	-0.24	2.47
Trp	0.00	1.14	4.07	-0.68	3.67	Trp	0.00	-2.90	2.00	-0.88	2.28
Cys	0.00	2.06	5.34	2.62	5.38	Cys	0.00	-1.53	4.38	1.01	4.37
Ser	0.00	2.53	5.67	2.35	4.54	Ser	0.00	-0.88	4.54	0.83	3.89
Thr	0.00	2.86	6.84	5.46	5.04	Thr	0.00	-0.91	6.66	4.43	4.38
Asn	0.00	0.15	2.09	2.23	4.43	Asn	0.00	-3.24	1.07	1.94	3.82
Gln	0.00	3.42	4.46	1.81	-0.85	Gln	0.00	0.55	3.13	0.03	-0.88
Asp	0.00	19.77	1.82	7.96	15.01	Asp	0.00	15.29	-1.49	6.74	14.13
Glu	0.00	7.46	2.38	4.26	9.08	Glu	0.00	3.29	-1.31	2.40	7.53
Lys	0.00	5.04	3.20	1.21	1.20	Lys	0.00	1.19	4.44	0.28	1.00
Arg	0.00	-3.03	-2.11	-17.77	-4.62	Arg	0.00	-6.15	-1.22	-19.40	-5.28

[a] AMBER99 dispersion correction

M05-2X-D[a]/6-31G**// M05-2X/6-31G**						PBE/cc-pVTZ//PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	1.94	9.95	12.57	5.54	Pro	0.00	2.14	-2.21	-0.41	-2.67
Gly	0.00	1.43	7.21	4.35	6.45	Gly	0.00	1.55	-3.07	-5.19	-1.10
Ala	0.00	1.93	6.94	4.31	5.99	Ala	0.00	2.27	-3.44	-5.45	-0.98
Val	0.00	4.18	5.36	2.87	6.22	Val	0.00	3.38	-4.38	-5.78	-0.95
Leu	0.00	3.34	6.86	3.37	6.44	Leu	0.00	2.87	-3.24	-5.47	-1.13
Ile	0.00	5.05	5.13	3.11	4.23	Ile	0.00	4.21	-4.41	-5.66	-1.41
Met	0.00	-0.65	6.45	3.91	4.49	Met	0.00	0.42	-3.25	-4.95	-1.42
Phe	0.00	-1.20	1.65	-0.15	5.77	Phe	0.00	-0.78	-5.32	-6.67	-2.06
Tyr	0.00	-0.99	0.79	-0.83	5.80	Tyr	0.00	-0.49	-5.15	-6.59	-2.08
His	0.00	-0.31	1.95	1.44	5.57	His	0.00	-0.49	-4.87	-6.19	-2.51
Trp	0.00	-0.05	6.19	1.32	6.23	Trp	0.00	-0.89	-4.73	-6.82	-2.69
Cys	0.00	0.32	7.36	4.21	7.49	Cys	0.00	1.29	-4.35	-4.69	0.25
Ser	0.00	1.27	7.68	4.07	6.50	Ser	0.00	1.53	-2.61	-5.06	-0.12
Thr	0.00	0.50	9.36	7.37	6.94	Thr	0.00	1.71	-1.29	-2.13	-0.12
Asn	0.00	-1.39	3.63	3.95	6.50	Asn	0.00	-0.16	-4.57	-4.11	-0.42
Gln	0.00	1.85	6.52	3.46	1.49	Gln	0.00	2.98	-3.63	-5.42	-4.07
Asp	0.00	18.07	1.44	8.28	16.93	Asp	0.00	16.24	-3.57	4.81	9.52
Glu	0.00	5.89	1.94	5.81	10.88	Glu	0.00	4.38	-5.72	-3.20	3.07
Lys	0.00	3.82	5.57	3.04	3.56	Lys	0.00	2.09	-3.38	-5.89	-3.44
Arg	0.00	-4.71	-0.42	-17.52	-2.45	Arg	0.00	-3.19	-7.08	-22.43	-8.14

[a] AMBER99 dispersion correction

PBE-D[a]/cc-pVTZ//PBE/6-31G**						PBE/6-31G**// PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	3.08	3.71	7.06	0.49	Pro	0.00	1.13	-0.40	1.52	0.41
Gly	0.00	2.75	0.06	-1.70	2.23	Gly	0.00	0.82	-0.57	-3.05	1.21
Ala	0.00	3.84	-0.19	-2.10	2.22	Ala	0.00	1.05	-1.03	-3.26	1.03
Val	0.00	6.27	-1.81	-2.76	2.34	Val	0.00	1.93	-1.80	-3.68	0.90
Leu	0.00	4.86	-0.59	-2.62	1.80	Leu	0.00	1.91	-0.42	-3.31	1.29
Ile	0.00	7.53	-1.97	-2.63	0.62	Ile	0.00	2.64	-1.84	-3.56	0.43
Met	0.00	2.07	-0.48	-2.08	1.05	Met	0.00	-0.93	-0.72	-2.77	0.56
Phe	0.00	1.41	-3.88	-5.08	1.22	Phe	0.00	-2.05	-3.26	-4.50	0.11
Tyr	0.00	1.66	-3.81	-5.00	1.40	Tyr	0.00	-1.79	-3.33	-4.47	0.05
His	0.00	1.60	-3.89	-4.51	0.60	His	0.00	-1.55	-2.61	-3.91	-0.17
Trp	0.00	1.96	-0.54	-4.61	1.26	Trp	0.00	-1.96	-2.27	-4.36	-0.31
Cys	0.00	3.14	-1.37	-1.48	3.37	Cys	0.00	-0.17	-1.92	-2.70	2.42
Ser	0.00	3.68	0.54	-1.82	2.49	Ser	0.00	0.48	-0.15	-2.88	1.92
Thr	0.00	3.12	1.41	0.81	2.45	Thr	0.00	-0.26	1.75	0.33	2.07
Asn	0.00	1.69	-2.01	-2.09	2.25	Asn	0.00	-1.60	-2.55	-2.02	1.64
Gln	0.00	4.28	-0.24	-1.99	-1.70	Gln	0.00	1.62	-1.15	-3.35	-1.74
Asp	0.00	19.01	-0.64	6.35	12.32	Asp	0.00	15.47	-3.65	6.14	11.83
Glu	0.00	6.98	-2.47	0.21	6.43	Glu	0.00	3.38	-5.57	-1.31	4.80
Lys	0.00	4.73	-2.25	-3.13	-0.88	Lys	0.00	1.16	-0.61	-3.56	-0.96
Arg	0.00	-1.75	-6.28	-20.55	-5.31	Arg	0.00	-4.86	-4.94	-22.37	-6.02

[a] AMBER99 dispersion correction

PBE-D[a]/6-31G**// PBE/6-31G**						B3LYP/cc-pVTZ//B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	2.07	5.52	8.99	3.57	Pro	0.00	2.42	-2.93	-1.38	-4.49
Gly	0.00	2.02	2.57	0.45	4.55	Gly	0.00	1.69	-4.08	-5.94	-2.86
Ala	0.00	2.63	2.21	0.10	4.24	Ala	0.00	2.58	-4.47	-6.74	-2.64
Val	0.00	4.82	0.77	-0.66	4.18	Val	0.00	3.71	-5.40	-6.88	-2.40
Leu	0.00	3.89	2.22	-0.46	4.21	Leu	0.00	3.11	-4.31	-6.64	-2.85
Ile	0.00	5.96	0.61	-0.53	2.47	Ile	0.00	4.62	-5.48	-6.76	-3.07
Met	0.00	0.73	2.05	0.11	3.03	Met	0.00	1.02	-4.28	-6.14	-2.71
Phe	0.00	0.14	-1.82	-2.90	3.39	Phe	0.00	-0.53	-6.08	-7.71	-3.79
Tyr	0.00	0.37	-1.99	-2.88	3.52	Tyr	0.00	-0.26	-6.08	-7.58	-3.87
His	0.00	0.54	-1.63	-2.23	2.93	His	0.00	-0.37	-5.61	-7.23	-4.26
Trp	0.00	0.89	1.92	-2.15	3.64	Trp	0.00	-0.90	-5.95	-8.09	-4.62
Cys	0.00	1.68	1.06	0.50	5.54	Cys	0.00	1.35	-5.35	-5.89	-1.55
Ser	0.00	2.63	2.99	0.36	4.53	Ser	0.00	1.47	-3.90	-6.50	-1.66
Thr	0.00	1.15	4.45	3.27	4.63	Thr	0.00	2.10	-2.49	-3.33	-1.75
Asn	0.00	0.24	0.01	0.00	4.31	Asn	0.00	-0.05	-5.70	-5.10	-2.13
Gln	0.00	2.92	2.24	0.07	0.63	Gln	0.00	3.54	-4.64	-6.61	-5.46
Asp	0.00	18.24	-0.71	7.68	14.63	Asp	0.00	17.18	-3.72	4.40	8.86
Glu	0.00	5.98	-2.32	2.11	8.15	Glu	0.00	4.60	-5.11	-4.13	1.78
Lys	0.00	3.80	0.53	-0.80	1.60	Lys	0.00	2.40	-4.45	-7.11	-5.27
Arg	0.00	-3.42	-4.14	-20.49	-3.19	Arg	0.00	-2.66	-7.97	-22.63	-9.99

[a] AMBER99 dispersion correction

B3LYP-D[a]/cc-pVTZ//B3LYP/6-31G**						B3LYP/6-31G**// B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	3.36	2.99	6.09	-1.33	Pro	0.00	1.50	-1.06	0.59	-1.38
Gly	0.00	2.89	-0.95	-2.45	0.48	Gly	0.00	1.01	-1.53	-3.59	-0.39
Ala	0.00	4.15	-1.23	-3.38	0.56	Ala	0.00	1.39	-2.04	-4.49	-0.43
Val	0.00	6.60	-2.83	-3.86	0.88	Val	0.00	2.38	-2.79	-4.71	-0.38
Leu	0.00	5.09	-1.66	-3.79	0.07	Leu	0.00	2.23	-1.47	-4.40	-0.24
Ile	0.00	7.93	-3.03	-3.73	-1.04	Ile	0.00	3.16	-2.87	-4.60	-0.97
Met	0.00	2.67	-1.51	-3.27	-0.24	Met	0.00	-0.29	-1.75	-3.94	-0.58
Phe	0.00	1.67	-4.64	-6.12	-0.51	Phe	0.00	-1.59	-3.90	-5.43	-1.41
Tyr	0.00	1.89	-4.74	-5.99	-0.39	Tyr	0.00	-1.34	-3.74	-5.34	-1.50
His	0.00	1.72	-4.63	-5.55	-1.15	His	0.00	-1.26	-3.21	-4.86	-1.68
Trp	0.00	1.95	-1.75	-5.89	-0.68	Trp	0.00	-1.77	-3.24	-5.53	-1.97
Cys	0.00	3.20	-2.38	-2.68	1.57	Cys	0.00	-0.03	-2.89	-3.87	0.77
Ser	0.00	3.62	-0.75	-3.26	0.95	Ser	0.00	0.47	-1.44	-4.29	0.49
Thr	0.00	3.51	0.21	-0.40	0.82	Thr	0.00	0.23	0.59	-0.80	0.58
Asn	0.00	1.80	-3.13	-3.08	0.54	Asn	0.00	-1.50	-3.69	-2.96	0.13
Gln	0.00	4.83	-1.25	-3.18	-3.09	Gln	0.00	2.19	-2.15	-4.51	-3.00
Asp	0.00	19.96	-0.79	5.94	11.66	Asp	0.00	16.39	-3.84	5.45	11.24
Glu	0.00	7.20	-1.86	-0.72	5.13	Glu	0.00	3.80	-4.67	-2.02	3.96
Lys	0.00	5.04	-3.31	-4.35	-2.70	Lys	0.00	1.59	-1.61	-4.68	-2.60
Arg	0.00	-1.22	-7.17	-20.76	-7.16	Arg	0.00	-4.20	-5.77	-22.45	-7.73

[a] AMBER99 dispersion correction

B3LYP-D[a]/6-31G**// B3LYP/6-31G**						AM1// AM1					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	2.44	4.86	8.07	1.78	Pro	0.00	3.31	-1.94	1.60	-1.55
Gly	0.00	2.21	1.60	-0.09	2.95	Gly	0.00	3.38	-2.81	-2.66	-1.85
Ala	0.00	2.97	1.21	-1.13	2.77	Ala	0.00	5.34	-2.33	-2.24	-1.53
Val	0.00	5.27	-0.22	-1.69	2.91	Val	0.00	6.77	-2.69	-2.08	-1.17
Leu	0.00	4.21	1.18	-1.55	2.69	Leu	0.00	4.36	-2.52	-3.24	-2.39
Ile	0.00	6.47	-0.42	-1.56	1.07	Ile	0.00	7.47	-2.62	-1.98	-2.46
Met	0.00	1.36	1.02	-1.07	1.89	Met	0.00	5.13	-1.14	-0.77	-0.08
Phe	0.00	0.61	-2.46	-3.84	1.88	Phe	0.00	1.09	-5.42	-4.54	-4.05
Tyr	0.00	0.81	-2.40	-3.75	1.98	Tyr	0.00	1.22	-5.34	-4.38	-4.12
His	0.00	0.83	-2.23	-3.17	1.42	His	0.00	1.10	-4.70	-3.72	-4.04
Trp	0.00	1.08	0.95	-3.32	1.97	Trp	0.00	0.66	-4.15	-4.69	-4.60
Cys	0.00	1.82	0.09	-0.67	3.88	Cys	0.00	3.79	-2.11	-1.67	0.01
Ser	0.00	2.62	1.70	-1.05	3.10	Ser	0.00	5.97	-0.53	1.29	-0.46
Thr	0.00	1.64	3.29	2.13	3.14	Thr	0.00	5.45	0.92	2.02	1.25
Asn	0.00	0.35	-1.13	-0.94	2.81	Asn	0.00	5.26	-1.24	-0.94	-0.24
Gln	0.00	3.49	1.24	-1.08	-0.63	Gln	0.00	6.70	-1.60	-1.41	-2.08
Asp	0.00	19.17	-0.91	6.99	14.04	Asp	0.00	21.23	-0.93	5.15	8.83
Glu	0.00	6.40	-1.42	1.39	7.32	Glu	0.00	5.26	-3.18	-2.75	0.69
Lys	0.00	4.22	-0.47	-1.92	-0.03	Lys	0.00	5.00	-2.14	-2.85	-3.90
Arg	0.00	-2.75	-4.97	-20.57	-4.90	Arg	0.00	0.70	-5.10	-12.02	-7.15

[a] AMBER99 dispersion correction

AM1-D[a]// AM1						PM3// PM3					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	4.25	3.98	9.07	1.61	Pro	0.00	4.04	-7.11	-5.93	-9.23
Gly	0.00	4.57	0.33	0.83	1.49	Gly	0.00	3.14	-4.79	-6.35	-9.98
Ala	0.00	6.91	0.91	1.12	1.68	Ala	0.00	4.75	-6.77	-7.15	-10.09
Val	0.00	9.66	-0.12	0.94	2.12	Val	0.00	5.70	-8.05	-7.80	-9.87
Leu	0.00	6.34	0.12	-0.39	0.54	Leu	0.00	2.85	-8.00	-8.65	-11.77
Ile	0.00	10.79	-0.17	1.05	-0.42	Ile	0.00	6.70	-7.84	-7.73	-10.74
Met	0.00	6.78	1.64	2.10	2.38	Met	0.00	5.09	-5.84	-6.09	-8.53
Phe	0.00	3.29	-3.98	-2.95	-0.77	Phe	0.00	1.39	-8.41	-8.91	-12.01
Tyr	0.00	3.37	-4.01	-2.80	-0.64	Tyr	0.00	1.55	-9.02	-8.78	-12.06
His	0.00	3.20	-3.72	-2.04	-0.93	His	0.00	2.36	-8.77	-8.42	-11.96
Trp	0.00	3.51	0.04	-2.49	-0.65	Trp	0.00	1.12	-7.86	-9.26	-12.64
Cys	0.00	5.64	0.87	1.54	3.13	Cys	0.00	3.46	-6.70	-5.82	-8.12
Ser	0.00	8.12	2.62	4.53	2.15	Ser	0.00	5.14	-1.93	-5.66	-7.07
Thr	0.00	6.86	3.62	4.96	3.82	Thr	0.00	2.93	-6.59	-6.45	-9.79
Asn	0.00	7.11	1.32	1.08	2.44	Asn	0.00	5.11	-4.98	-5.12	-8.23
Gln	0.00	8.00	1.79	2.02	0.29	Gln	0.00	6.25	-6.18	-6.32	-10.20
Asp	0.00	24.00	2.01	6.69	11.63	Asp	0.00	20.33	-5.20	-3.56	0.62
Glu	0.00	7.86	0.07	0.66	4.04	Glu	0.00	4.14	-7.12	-7.32	-6.69
Lys	0.00	7.64	-1.00	-0.09	-1.34	Lys	0.00	5.46	-6.85	-7.63	-12.11
Arg	0.00	2.14	-4.30	-10.15	-4.32	Arg	0.00	1.77	-9.69	-17.60	-14.32

[a] AMBER99 dispersion correction

PM3-D[a]// PM3						PM3MM// PM3MM					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	4.98	-1.19	1.54	-6.07	Pro	0.00	4.57	-7.64	-6.21	-8.75
Gly	0.00	4.33	-1.65	-2.85	-6.64	Gly	0.00	3.57	-7.73	-7.80	-9.53
Ala	0.00	6.33	-3.52	-3.79	-6.89	Ala	0.00	5.45	-7.71	-7.95	-9.43
Val	0.00	8.59	-5.48	-4.78	-6.58	Val	0.00	6.45	-8.68	-8.21	-9.14
Leu	0.00	4.83	-5.36	-5.80	-8.85	Leu	0.00	3.71	-8.76	-9.10	-10.98
Ile	0.00	10.02	-5.39	-4.70	-8.70	Ile	0.00	7.34	-8.58	-8.21	-9.98
Met	0.00	6.74	-3.06	-3.21	-6.06	Met	0.00	5.44	-6.77	-6.81	-7.81
Phe	0.00	3.58	-6.97	-7.32	-8.72	Phe	0.00	2.15	-10.09	-9.45	-11.48
Tyr	0.00	3.70	-7.68	-7.19	-8.59	Tyr	0.00	2.29	-9.96	-9.25	-11.54
His	0.00	4.46	-7.79	-6.74	-8.85	His	0.00	2.91	-9.31	-8.67	-11.45
Trp	0.00	3.97	-3.67	-7.06	-8.69	Trp	0.00	1.86	-8.79	-9.50	-12.12
Cys	0.00	5.31	-3.72	-2.61	-5.00	Cys	0.00	3.95	-7.90	-8.01	-7.80
Ser	0.00	7.29	1.22	-2.42	-4.46	Ser	0.00	6.15	-6.42	-4.74	-8.35
Thr	0.00	4.34	-3.89	-3.51	-7.22	Thr	0.00	3.88	-7.88	-9.55	-8.88
Asn	0.00	6.96	-2.42	-3.11	-5.55	Asn	0.00	5.33	-7.39	-6.49	-8.31
Gln	0.00	7.55	-2.80	-2.89	-7.83	Gln	0.00	6.95	-7.29	-7.59	-9.93
Asp	0.00	23.11	-2.26	-2.02	3.42	Asp	0.00	17.61	-4.05	-2.19	0.52
Glu	0.00	6.74	-3.87	-3.91	-3.33	Glu	0.00	6.73	-6.70	-6.66	-5.26
Lys	0.00	8.09	-5.71	-4.87	-9.54	Lys	0.00	5.35	-8.89	-9.50	-12.46
Arg	0.00	3.22	-8.90	-15.73	-11.49	Arg	0.00	1.22	-12.15	-19.96	-15.27

[a] AMBER99 dispersion correction

PM3MM-D[a]// PM3MM						AMOEBA// AMOEBA					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	5.51	-1.72	1.26	-5.59	Pro	0.00	1.61	9.86	14.31	1.46
Gly	0.00	4.77	-4.59	-4.30	-6.19	Gly	0.00	0.99	3.94	1.99	1.44
Ala	0.00	7.02	-4.46	-4.59	-6.22	Ala	0.00	1.25	3.48	1.23	1.39
Val	0.00	9.34	-6.11	-5.19	-5.85	Val	0.00	2.63	3.38	2.12	0.84
Leu	0.00	5.69	-6.11	-6.25	-8.06	Leu	0.00	2.46	3.47	1.99	1.88
Ile	0.00	10.66	-6.14	-5.18	-7.94	Ile	0.00	3.07	3.26	2.25	1.67
Met	0.00	7.09	-4.00	-3.94	-5.34	Met	0.00	0.13	4.12	1.75	1.37
Phe	0.00	4.35	-8.65	-7.86	-8.19	Phe	0.00	-1.07	1.31	0.13	2.69
Tyr	0.00	4.45	-8.63	-7.66	-8.06	Tyr	0.00	-1.22	0.72	-0.33	2.48
His	0.00	5.01	-8.33	-6.99	-8.34	His	0.00	-2.89	-1.80	-3.12	-1.80
Trp	0.00	4.72	-4.60	-7.29	-8.17	Trp	0.00	-1.52	3.28	0.05	0.49
Cys	0.00	5.80	-4.92	-4.80	-4.68	Cys	0.00	-0.93	0.71	0.62	1.65
Ser	0.00	8.30	-3.27	-1.50	-5.74	Ser	0.00	-0.44	5.33	1.94	4.41
Thr	0.00	5.29	-5.17	-6.61	-6.32	Thr	0.00	1.62	3.29	2.65	-1.32
Asn	0.00	7.18	-4.83	-4.48	-5.64	Asn	0.00	-1.94	-0.49	-2.92	1.49
Gln	0.00	8.24	-3.91	-4.16	-7.56	Gln	0.00	3.14	2.04	-0.06	-2.02
Asp	0.00	20.39	-1.12	-0.64	3.33	Asp	0.00	12.41	4.99	7.37	11.94
Glu	0.00	9.33	-3.45	-3.25	-1.90	Glu	0.00	3.87	3.38	5.10	5.67
Lys	0.00	7.98	-7.75	-6.74	-9.90	Lys	0.00	-0.50	1.19	-0.58	-2.87
Arg	0.00	2.66	-11.35	-18.09	-12.44	Arg	0.00	-3.11	0.08	-16.95	-5.49

[a] AMBER99 dispersion correction

AMBEREP// AMBEREP					
	α_R	α_L	β	β_a	PPII
Pro	0.00	51.32	11.11	12.11	4.41
Gly	0.00	7.37	3.05	-0.16	4.71
Ala	0.00	11.42	5.05	1.84	4.75
Val	0.00	11.25	3.02	0.31	4.09
Leu	0.00	12.23	5.46	1.11	4.92
Ile	0.00	14.42	3.48	0.71	3.17
Met	0.00	9.55	5.50	2.35	5.07
Phe	0.00	9.31	2.25	0.03	4.51
Tyr	0.00	8.93	1.48	-0.70	4.50
His	0.00	5.51	-0.09	-0.75	1.84
Trp	0.00	11.61	6.42	1.91	5.25
Cys	0.00	11.47	7.06	3.31	5.28
Ser	0.00	9.96	5.92	1.69	5.86
Thr	0.00	11.63	7.58	5.75	3.51
Asn	0.00	10.82	3.90	-0.07	5.60
Gln	0.00	10.70	4.54	1.44	-0.66
Asp	0.00	20.54	3.00	6.67	15.75
Glu	0.00	18.62	7.19	5.90	12.90
Lys	0.00	11.91	3.75	0.24	1.44
Arg	0.00	5.28	-0.53	-13.93	-3.50

AMBERPOL// AMBERPOL					
	α_R	α_L	β	β_a	PPII
Pro	0.00	8.11	12.69	14.13	3.58
Gly	0.00	7.13	4.54	2.34	2.22
Ala	0.00	11.09	6.32	3.54	3.19
Val	0.00	10.51	3.99	1.83	2.76
Leu	0.00	11.79	6.57	2.61	3.57
Ile	0.00	13.97	4.76	2.47	1.84
Met	0.00	10.07	6.63	4.01	3.66
Phe	0.00	8.70	3.15	1.41	3.19
Tyr	0.00	9.00	2.63	1.15	2.94
His	0.00	6.70	1.68	0.99	1.28
Trp	0.00	10.70	7.54	3.29	3.87
Cys	0.00	9.88	6.28	3.12	3.90
Ser	0.00	9.04	6.52	2.73	4.20
Thr	0.00	13.99	8.74	7.43	4.30
Asn	0.00	8.81	3.42	0.22	3.48
Gln	0.00	10.18	5.38	2.78	-2.17
Asp	0.00	19.09	3.10	7.13	13.64
Glu	0.00	17.50	7.72	7.12	10.92
Lys	0.00	11.67	4.44	2.14	0.62
Arg	0.00	6.03	0.91	-12.19	-3.92

AMBER94// AMBER94					
	α_R	α_L	β	β_a	PPII
Pro	0.00	8.42	11.52	16.08	5.30
Gly	0.00	7.82	6.77	5.16	4.36
Ala	0.00	12.36	8.39	6.28	5.01
Val	0.00	12.10	6.13	4.49	4.89
Leu	0.00	13.14	7.54	6.56	6.02
Ile	0.00	12.82	5.87	4.49	2.20
Met	0.00	9.25	8.41	6.17	5.25
Phe	0.00	10.09	5.27	4.25	5.17
Tyr	0.00	9.42	4.54	3.81	4.74
His	0.00	9.46	5.81	5.88	4.64
Trp	0.00	10.01	8.60	5.10	5.00
Cys	0.00	9.44	9.24	6.63	5.88
Ser	0.00	7.70	9.44	6.37	4.93
Thr	0.00	12.14	9.66	9.02	7.70
Asn	0.00	6.57	3.44	5.29	4.94
Gln	0.00	13.64	8.34	6.16	0.59
Asp	0.00	23.34	7.40	12.51	18.19
Glu	0.00	17.86	10.60	9.38	13.51
Lys	0.00	11.76	7.88	5.81	1.67
Arg	0.00	6.22	3.64	-8.18	-3.48

AMBER96// AMBER96					
	α_R	α_L	β	β_a	PPII
Pro	0.00	8.42	2.96	6.10	-0.49
Gly	0.00	7.82	-1.79	-4.82	-1.44
Ala	0.00	12.36	-0.17	-3.69	-0.78
Val	0.00	12.10	-2.43	-5.49	-0.91
Leu	0.00	13.14	-1.02	-3.41	0.22
Ile	0.00	12.82	-2.69	-5.49	-3.59
Met	0.00	9.25	-0.15	-3.81	-0.54
Phe	0.00	10.09	-3.29	-5.73	-0.62
Tyr	0.00	9.43	-4.02	-6.16	-1.06
His	0.00	9.46	-2.75	-4.10	-1.15
Trp	0.00	10.01	0.04	-4.88	-0.79
Cys	0.00	9.44	0.68	-3.35	0.08
Ser	0.00	7.70	0.88	-3.61	-0.86
Thr	0.00	12.14	1.10	-0.96	1.90
Asn	0.00	6.57	-5.12	-4.69	-0.85
Gln	0.00	13.64	-0.22	-3.82	-5.20
Asp	0.00	23.34	-1.16	2.53	12.40
Glu	0.00	17.86	2.04	-0.60	7.71
Lys	0.00	11.76	-0.68	-4.17	-4.12
Arg	0.00	6.22	-4.92	-18.15	-9.27

AMBER99// AMBER99					
	α_R	α_L	β	β_a	PPII
Pro	0.00	6.39	10.33	11.20	5.01
Gly	0.00	5.81	6.34	0.77	4.28
Ala	0.00	9.38	7.22	1.46	4.73
Val	0.00	9.08	4.94	-0.34	4.60
Leu	0.00	10.17	6.36	1.82	5.76
Ile	0.00	9.62	4.64	-0.39	1.88
Met	0.00	6.25	7.22	1.33	4.98
Phe	0.00	7.11	4.09	-0.58	4.89
Tyr	0.00	6.45	3.36	-1.01	4.45
His	0.00	6.48	4.62	1.06	4.37
Trp	0.00	7.04	7.41	0.27	4.72
Cys	0.00	6.45	8.07	1.82	5.59
Ser	0.00	4.69	8.28	1.56	4.68
Thr	0.00	9.02	8.47	4.18	7.41
Asn	0.00	3.56	2.25	1.22	4.67
Gln	0.00	11.35	7.17	1.34	0.97
Asp	0.00	20.20	6.42	7.68	17.90
Glu	0.00	15.25	9.42	4.56	13.24
Lys	0.00	8.81	6.68	0.96	1.37
Arg	0.00	3.32	2.44	-12.82	-3.78

AMBER99SB// AMBER99SB					
	α_R	α_L	β	β_a	PPII
Pro	0.00	2.77	4.22	4.50	-3.75
Gly	0.00	1.58	0.71	-2.98	-3.40
Ala	0.00	3.08	0.38	-3.78	-3.43
Val	0.00	2.78	-1.90	-5.60	-3.61
Leu	0.00	3.91	-0.47	-3.42	-2.39
Ile	0.00	3.33	-2.19	-5.64	-6.47
Met	0.00	-0.03	0.39	-3.90	-3.15
Phe	0.00	0.83	-2.73	-5.80	-3.23
Tyr	0.00	0.16	-3.45	-6.20	-3.69
His	0.00	0.17	-2.22	-4.18	-3.90
Trp	0.00	0.77	0.57	-4.92	-3.44
Cys	0.00	0.18	1.07	-3.41	-2.48
Ser	0.00	-1.58	1.41	-3.73	-3.50
Thr	0.00	1.84	1.04	-1.67	-1.93
Asn	0.00	-2.52	-4.48	-3.64	-3.36
Gln	0.00	5.92	0.36	-3.90	-6.56
Asp	0.00	13.93	-0.30	2.54	9.79
Glu	0.00	8.76	2.60	-0.69	5.03
Lys	0.00	2.58	-0.14	-4.29	-6.81
Arg	0.00	-2.93	-4.38	-17.99	-11.98

AMBER03// AMBER03					
	α_R	α_L	β	β_a	PPII
Pro	0.00	9.90	7.51	5.76	-1.82
Gly	0.00	8.39	1.96	-0.91	-1.23
Ala	0.00	13.55	2.44	-1.43	-1.28
Val	0.00	10.51	-0.97	-4.48	-1.35
Leu	0.00	14.37	1.89	-0.98	-0.89
Ile	0.00	14.77	-2.36	-5.55	-5.37
Met	0.00	9.41	3.55	-0.43	-0.93
Phe	0.00	9.73	0.43	-2.22	-0.38
Tyr	0.00	11.86	3.34	1.00	2.43
His	0.00	11.46	5.12	3.46	2.48
Trp	0.00	10.76	5.23	1.26	2.43
Cys	0.00	10.24	3.66	-0.55	-0.22
Ser	0.00	11.29	3.46	-1.54	-0.65
Thr	0.00	12.68	1.75	0.25	-3.68
Asn	0.00	6.19	-0.84	0.28	0.33
Gln	0.00	16.82	-0.81	-5.12	-7.59
Asp	0.00	25.97	3.59	5.55	14.11
Glu	0.00	17.18	1.67	-2.60	3.68
Lys	0.00	5.15	-2.27	-5.34	-9.72
Arg	0.00	2.62	-2.54	-12.79	-10.80

CHARMM27// CHARMM27					
	α_R	α_L	β	β_a	PPII
Pro	0.00	13.34	5.21	7.31	-2.51
Gly	0.00	13.21	-1.21	-2.21	-0.90
Ala	0.00	20.28	1.75	0.67	-0.53
Val	0.00	21.74	0.06	0.04	-0.45
Leu	0.00	19.86	0.67	0.42	-1.16
Ile	0.00	22.58	-0.08	0.10	-2.27
Met	0.00	18.41	1.53	0.37	-0.82
Phe	0.00	15.52	-2.83	-2.73	-2.67
Tyr	0.00	15.48	-3.25	-2.95	-2.87
His	0.00	11.91	-2.56	-1.90	-3.91
Trp	0.00	16.21	0.10	-1.41	-1.71
Cys	0.00	17.63	1.57	0.46	-0.41
Ser	0.00	16.24	2.18	0.12	2.27
Thr	0.00	20.99	2.62	3.53	1.19
Asn	0.00	16.71	0.84	-0.64	-0.80
Gln	0.00	21.90	1.34	0.23	-4.22
Asp	0.00	38.08	10.54	11.94	14.49
Glu	0.00	26.89	6.07	6.37	7.91
Lys	0.00	18.59	-0.13	-1.03	-4.51
Arg	0.00	12.97	-4.56	-14.61	-10.39

OPLS-AA// OPLS-AA					
	α_R	α_L	β	β_a	PPII
Pro	0.00	3.09	3.54	12.46	-2.43
Gly	0.00	3.62	-1.19	-3.05	-1.12
Ala	0.00	5.83	-1.60	-3.20	-1.57
Val	0.00	6.60	-2.99	-3.98	-2.03
Leu	0.00	5.44	-2.62	-3.79	-2.17
Ile	0.00	7.54	-3.22	-3.96	-4.99
Met	0.00	5.20	-2.07	-3.79	0.81
Phe	0.00	0.10	-6.09	-6.24	-3.78
Tyr	0.00	0.07	-6.46	-6.41	-3.95
His	0.00	0.76	-4.71	-4.52	-3.46
Trp	0.00	4.47	-2.88	-2.65	-0.76
Cys	0.00	2.21	-2.90	-4.24	-1.07
Ser	0.00	2.21	-1.71	-4.18	-0.56
Thr	0.00	3.17	-0.12	-0.11	-2.82
Asn	0.00	-2.32	-8.79	-3.64	-1.58
Gln	0.00	4.93	-0.55	-2.33	-7.70
Asp	0.00	14.77	-3.64	9.03	12.51
Glu	0.00	9.86	1.98	0.19	4.70
Lys	0.00	4.01	-4.57	-6.18	-6.59
Arg	0.00	0.14	-7.13	-17.02	-10.92

OPLS-AA/L// OPLS-AA/L					
	α_R	α_L	β	β_a	PPII
Pro	0.00	4.02	4.66	13.19	-3.77
Gly	0.00	4.47	-6.20	-8.06	-3.52
Ala	0.00	7.14	-0.02	-3.09	-2.40
Val	0.00	7.90	-1.36	-3.86	-2.40
Leu	0.00	6.33	-0.95	-3.84	-3.40
Ile	0.00	9.03	-1.57	-3.80	-2.39
Met	0.00	6.55	-0.62	-3.71	-0.02
Phe	0.00	1.39	-4.52	-5.90	-4.68
Tyr	0.00	1.33	-4.91	-6.03	-4.84
His	0.00	1.20	-3.37	-4.27	-4.30
Trp	0.00	4.83	-1.37	-3.03	-2.18
Cys	0.00	3.63	-2.60	-5.50	-1.89
Ser	0.00	3.62	-0.09	-4.38	-5.04
Thr	0.00	5.03	1.54	0.29	-3.00
Asn	0.00	1.74	-3.93	-5.43	-2.73
Gln	0.00	6.50	-0.81	-3.53	-7.65
Asp	0.00	20.51	3.89	10.44	13.03
Glu	0.00	15.09	3.70	4.08	7.59
Lys	0.00	5.99	-2.22	-5.15	-6.53
Arg	0.00	0.79	-5.87	-17.37	-12.09

AMBERUA// AMBERUA					
	α_R	α_L	β	β_a	PPII
Pro	0.00	55.22	5.40	7.20	-2.92
Gly	0.00	10.62	1.65	-1.42	-1.26
Ala	0.00	16.62	4.73	0.82	0.77
Val	0.00	11.95	1.88	-1.42	-1.72
Leu	0.00	17.60	4.72	1.17	1.54
Ile	0.00	15.78	3.12	-0.06	-0.77
Met	0.00	12.09	4.54	0.93	0.43
Phe	0.00	13.25	1.69	-1.18	0.28
Tyr	0.00	15.97	5.34	2.78	4.17
His	0.00	13.62	3.31	1.23	0.67
Trp	0.00	14.10	5.97	1.30	1.69
Cys	0.00	14.04	5.59	1.50	1.83
Ser	0.00	13.23	6.50	1.79	4.70
Thr	0.00	17.71	4.31	1.89	2.56
Asn	0.00	9.58	-0.88	-0.04	-0.08
Gln	0.00	16.89	3.27	-0.82	-5.87
Asp	0.00	28.58	3.09	7.49	13.20
Glu	0.00	18.20	4.05	0.98	5.68
Lys	0.00	14.22	4.67	0.91	-1.66
Arg	0.00	5.47	-1.65	-12.97	-9.12

GROMOS(G43b1)// GROMOS(G43b1)					
	α_R	α_L	β	β_a	PPII
Pro	0.00	44.79	0.67	5.04	-3.81
Gly	0.00	4.14	-5.30	-4.95	-3.11
Ala	0.00	6.46	-5.27	-4.97	-2.93
Val	0.00	6.24	-6.22	-5.12	-3.59
Leu	0.00	5.79	-5.70	-5.76	-3.18
Ile	0.00	7.63	-6.27	-4.99	-4.21
Met	0.00	5.84	-5.07	-4.52	-3.10
Phe	0.00	4.87	-7.96	-7.25	-2.74
Tyr	0.00	4.92	-8.21	-7.89	-2.51
His	0.00	5.11	-6.48	-5.53	-3.96
Trp	0.00	6.90	-2.68	-4.73	-1.99
Cys	0.00	5.77	-5.41	-5.21	-3.08
Ser	0.00	6.08	-3.40	-3.93	-0.77
Thr	0.00	4.14	-3.05	-1.94	-2.14
Asn	0.00	4.40	-6.38	-6.34	-3.07
Gln	0.00	7.34	-4.62	-4.19	-7.52
Asp	0.00	-0.68	-7.73	-6.83	-7.50
Glu	0.00	6.04	2.47	-5.06	-3.50
Lys	0.00	4.93	-6.96	-6.13	-4.16
Arg	0.00	7.10	-4.59	-5.20	-2.88

GROMOS(G45a3)// GROMOS(G45a3)						GROMOS(G53a6)// GROMOS(G53a6)					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.00	42.57	-0.42	3.85	-4.43	Pro	0.00	44.77	-0.21	16.41	-6.06
Gly	0.00	2.45	-5.74	-5.37	-3.23	Gly	0.00	2.36	-8.57	-8.69	-5.15
Ala	0.00	3.93	-5.84	-5.52	-2.98	Ala	0.00	3.92	-8.67	-8.81	-4.97
Val	0.00	5.36	-6.64	-5.36	-3.56	Val	0.00	5.64	-9.51	-8.45	-5.26
Leu	0.00	3.39	-6.44	-5.75	-3.01	Leu	0.00	3.12	-9.46	-9.02	-6.23
Ile	0.00	6.27	-6.61	-5.05	-3.61	Ile	0.00	6.61	-9.47	-8.11	-5.78
Met	0.00	4.20	-5.51	-4.85	-2.92	Met	0.00	2.02	-6.96	-6.81	-3.59
Phe	0.00	2.75	-8.68	-7.84	-2.98	Phe	0.00	1.85	-11.63	-10.88	-5.42
Tyr	0.00	2.91	-8.85	-8.13	-2.64	Tyr	0.00	2.07	-11.80	-11.18	-5.05
His	0.00	3.04	-7.07	-5.31	-4.14	His	0.00	2.77	-10.45	-7.78	-5.19
Trp	0.00	4.81	-3.18	-5.21	-2.29	Trp	0.00	4.04	-6.31	-8.09	-5.03
Cys	0.00	3.79	-5.93	-5.62	-3.14	Cys	0.00	1.78	-8.33	-8.83	-4.35
Ser	0.00	4.08	-3.90	-4.35	-0.77	Ser	0.00	3.00	-6.17	-7.26	-4.04
Thr	0.00	3.27	-3.58	-2.22	-1.81	Thr	0.00	4.26	-5.49	-4.13	-5.39
Asn	0.00	2.45	-6.82	-6.79	-3.13	Asn	0.00	2.43	-9.75	-7.49	-4.91
Gln	0.00	5.79	-5.17	-4.56	-6.96	Gln	0.00	7.54	-7.45	-7.36	-9.85
Asp	0.00	17.26	0.92	-1.14	2.00	Asp	0.00	20.61	-1.39	-1.65	3.44
Glu	0.00	8.07	5.54	-3.62	-0.88	Glu	0.00	7.56	0.40	-6.29	-1.32
Lys	0.00	2.32	-6.68	-5.20	-3.77	Lys	0.00	2.94	-8.83	-8.08	-6.30
Arg	0.00	-1.14	-8.73	-11.09	-7.22	Arg	0.00	-1.74	-12.16	-16.21	-10.85

Table S3a. Energy offset (E_c) (kcal/mol) for each tetrapeptide obtained from Eq. 2 in minimizing RMS over the 5 conformations.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg
M05-2X/cc-pVTZ	1.12	1.34	1.25	1.19	1.14	1.14	1.06	1.59	1.69	1.45	1.90	0.74	1.21	1.01	1.16	1.01	0.35	0.85	1.22	1.14
M05-2X-D[a]/cc-pVTZ	-2.38	-0.89	-1.02	-1.17	-0.94	-1.03	-0.89	-0.11	-0.03	-0.12	-0.74	-1.49	-1.02	-0.91	-0.66	-1.09	-1.66	-1.67	-0.60	-0.25
M05-2X/6-31G**	0.21	0.31	0.36	0.45	0.16	0.37	0.18	0.83	1.05	0.60	0.80	-0.06	0.32	0.22	0.40	0.11	0.32	0.58	0.15	0.65
M05-2X-D[a]/6-31G**	-3.29	-1.92	-1.92	-1.90	-1.92	-1.80	-1.77	-0.87	-0.66	-0.98	-1.84	-2.29	-1.91	-1.70	-1.42	-1.99	-1.70	-1.94	-1.67	-0.74
PBE/cc-pVTZ	3.34	3.53	3.44	3.37	3.47	3.16	2.91	3.31	3.16	3.57	3.92	3.09	3.25	3.50	2.97	2.70	1.85	3.26	3.65	2.41
PBE-D[a]/cc-pVTZ	-0.16	1.29	1.16	1.01	1.39	1.00	0.95	1.60	1.45	2.00	1.28	0.86	1.02	1.57	1.15	0.61	-0.16	0.74	1.84	1.02
PBE/6-31G**	2.18	2.28	2.36	2.35	2.19	2.17	1.84	2.28	2.20	2.40	2.67	2.06	2.12	2.35	2.02	1.60	1.29	2.70	2.32	1.88
PBE-D[a]/6-31G**	-1.32	0.05	0.08	0.00	0.11	0.01	-0.12	0.58	0.49	0.83	0.04	-0.17	-0.11	0.43	0.20	-0.50	-0.72	0.18	0.50	0.49
B3LYP/cc-pVTZ	3.99	4.20	4.17	4.02	4.22	3.85	3.49	3.96	3.85	4.25	4.81	3.88	4.11	4.23	3.71	3.31	1.91	3.54	4.41	2.90
B3LYP-D[a]/cc-pVTZ	0.49	1.97	1.89	1.66	2.14	1.68	1.54	2.26	2.14	2.68	2.17	1.65	1.88	2.30	1.89	1.21	-0.11	1.01	2.59	1.51
B3LYP/6-31G**	2.78	2.86	3.03	2.92	2.86	2.76	2.38	2.81	2.68	2.96	3.40	2.80	2.95	3.01	2.72	2.17	1.40	2.75	2.99	2.27
B3LYP-D[a]/6-31G**	-0.72	0.63	0.75	0.57	0.78	0.59	0.43	1.10	0.97	1.39	0.76	0.56	0.72	1.09	0.90	0.07	-0.61	0.23	1.17	0.88
AM1	2.43	2.75	2.07	1.65	2.84	1.62	0.44	2.92	2.82	3.03	3.45	1.58	0.74	1.21	0.55	0.35	0.39	2.96	2.30	-1.04
AM1-D[a]	-1.07	0.52	-0.21	-0.70	0.76	-0.54	-1.51	1.22	1.11	1.45	0.81	-0.65	-1.49	-0.72	-1.27	-1.74	-1.62	0.44	0.49	-2.43
PM3	6.36	5.56	5.77	5.82	7.20	5.63	4.14	5.93	5.96	6.11	6.62	5.03	3.90	7.11	3.76	3.97	4.81	6.36	5.75	2.22
PM3-D[a]	2.86	3.33	3.49	3.47	5.12	3.46	2.19	4.23	4.25	4.54	3.99	2.80	1.67	5.19	1.94	1.87	2.80	3.84	3.94	0.82
PM3MM	6.31	6.26	5.84	5.74	7.11	5.59	4.26	6.12	5.99	6.06	6.60	5.54	4.67	7.62	4.49	4.25	4.87	5.34	6.63	3.48
PM3MM-D[a]	2.82	4.03	3.57	3.38	5.03	3.43	2.30	4.41	4.28	4.49	3.96	3.31	2.44	5.69	2.67	2.15	2.86	2.82	4.81	2.09
AMOEBA	-2.74	0.29	0.45	0.03	0.12	-0.34	-0.41	-0.27	-0.03	2.68	0.43	1.18	-0.25	1.88	1.89	0.06	-0.09	-0.64	2.08	-0.66
AMBEREP	-13.08	-1.03	-2.70	-1.91	-2.66	-2.65	-3.43	-2.88	-2.55	-0.55	-4.14	-3.84	-2.69	-2.56	-2.93	-2.53	-1.94	-5.96	-1.94	-3.22
AMBERPOL	-4.99	-1.28	-2.91	-2.00	-2.83	-2.90	-3.81	-2.95	-2.85	-1.37	-4.18	-3.05	-2.50	-3.76	-2.07	-2.56	-1.35	-5.69	-2.25	-3.92
AMBER94	-5.55	-2.86	-4.49	-3.70	-4.57	-3.37	-4.75	-4.62	-4.21	-4.40	-4.85	-4.65	-3.69	-4.57	-2.93	-5.07	-5.04	-7.30	-3.90	-5.40
AMBER96	-0.69	2.01	0.37	1.17	0.29	1.50	0.12	0.25	0.66	0.46	0.02	0.22	1.18	0.30	1.93	-0.20	-0.17	-2.44	0.97	-0.53
AMBER99	-3.87	-1.48	-2.64	-1.83	-2.74	-1.44	-2.89	-2.76	-2.35	-2.55	-2.99	-2.80	-1.85	-2.68	-1.23	-3.49	-3.19	-5.53	-2.04	-3.59
AMBER99SB	-1.92	2.78	2.67	3.49	2.55	3.90	2.41	2.53	2.93	2.78	2.30	2.52	3.47	3.28	3.92	1.51	2.05	-0.17	3.26	1.70
AMBER03	-1.56	0.32	-0.74	1.08	-0.80	1.41	-1.25	-1.17	-3.43	-3.75	-3.04	-1.04	-0.52	0.93	-0.08	0.02	-2.60	-1.02	3.96	-1.05
CHARMM27	-1.96	0.18	-2.52	-2.46	-1.88	-2.36	-2.83	-1.12	-0.99	0.05	-1.74	-2.26	-2.16	-2.53	-2.11	-3.17	-7.76	-6.48	-1.06	-2.44
OPLS-AA	-0.62	2.31	2.02	2.30	2.71	2.63	1.04	3.54	3.65	3.14	1.26	2.79	2.84	3.11	4.38	1.81	0.71	-0.38	4.19	1.23
OPLS-AA/L	-0.91	4.62	1.59	1.77	2.45	1.45	0.63	3.08	3.19	2.90	1.25	2.86	3.17	2.36	3.19	1.77	-2.33	-3.13	3.11	1.15
AMBERUA	-10.27	0.04	-2.67	-0.32	-2.93	-1.91	-2.53	-2.47	-5.36	-3.01	-3.71	-3.00	-3.25	-2.16	-0.60	-2.02	-3.22	-2.82	-2.10	-2.10
GROMOS(G43b1)	-6.63	3.81	3.26	3.56	3.85	3.28	2.44	2.96	3.03	2.93	1.40	3.18	2.40	3.73	3.39	2.48	11.79	2.98	3.99	-4.64
GROMOS(G45a3)	-5.60	4.34	4.00	3.86	4.44	3.51	2.88	3.69	3.64	3.45	2.07	3.77	2.98	4.00	3.97	2.86	3.44	1.14	4.19	-0.12
GROMOS(G53a6)	-8.27	5.97	5.62	5.33	6.40	5.06	4.13	5.56	5.49	4.89	3.97	5.54	4.89	5.28	5.06	4.10	3.04	2.90	5.58	2.44

[a] AMBER99 dispersion correction.

Table S3b. Signed error ($error = E_{ai} - E_{bi} + E_c$) using the MP2 energy as the true value.

M05-2X/cc-pVTZ//M05-2X/6-31G**						M05-2X-D[a]/cc-pVTZ//M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	1.12	1.11	-0.55	-0.62	-1.06	Pro	-2.38	-1.44	1.87	3.35	-1.40
Gly	1.34	0.95	-0.36	-1.33	-0.61	Gly	-0.89	-0.09	0.54	-0.06	0.50
Ala	1.25	0.71	-0.43	-0.65	-0.89	Ala	-1.02	0.02	0.54	0.43	0.04
Val	1.19	0.73	-0.25	-0.83	-0.84	Val	-1.17	1.27	-0.04	-0.16	0.10
Leu	1.14	0.63	-0.28	-0.83	-0.66	Leu	-0.94	0.54	0.28	-0.06	0.18
Ile	1.14	0.61	-0.27	-0.78	-0.70	Ile	-1.03	1.76	0.01	0.08	-0.83
Met	1.06	0.43	-0.37	-0.63	-0.50	Met	-0.89	0.13	0.45	0.30	0.02
Phe	1.59	0.28	-0.25	-0.76	-0.86	Phe	-0.11	0.78	-0.51	-0.87	0.72
Tyr	1.69	0.49	-0.63	-0.88	-0.66	Tyr	-0.03	0.93	-1.01	-1.00	1.11
His	1.45	0.24	-0.36	-0.57	-0.76	His	-0.12	0.76	-0.95	-0.46	0.77
Trp	1.90	0.38	-0.76	-0.72	-0.78	Trp	-0.74	0.59	0.79	-1.15	0.52
Cys	0.74	0.00	1.32	-1.00	-1.06	Cys	-1.49	-0.38	2.07	-0.02	-0.17
Ser	1.21	0.26	-0.17	-0.81	-0.48	Ser	-1.02	0.18	0.75	0.20	-0.10
Thr	1.01	0.48	-0.29	-0.68	-0.51	Thr	-0.91	-0.04	0.49	0.33	0.13
Asn	1.16	0.29	-0.68	-0.16	-0.61	Asn	-0.66	0.32	0.06	0.03	0.24
Gln	1.01	1.07	-0.56	-1.05	-0.47	Gln	-1.09	0.27	0.73	0.28	-0.20
Asp	0.35	0.63	-0.32	-0.24	-0.42	Asp	-1.66	1.40	0.60	-0.71	0.38
Glu	0.85	0.37	0.61	-1.21	-0.62	Glu	-1.67	0.45	1.34	-0.33	0.21
Lys	1.22	0.70	-0.23	-0.75	-0.93	Lys	-0.60	1.51	-0.91	0.19	-0.19
Arg	1.14	0.72	-0.43	-0.02	-1.42	Arg	-0.25	0.78	-1.03	0.47	0.03

[a] AMBER99 dispersion correction.

M05-2X/6-31G**// M05-2X/6-31G**						M05-2X-D/6-31G**// M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.21	-1.04	-0.02	0.01	0.83	Pro	-3.29	-3.59	2.40	3.99	0.49
Gly	0.31	-1.01	0.72	-0.58	0.57	Gly	-1.92	-2.05	1.62	0.68	1.67
Ala	0.36	-1.51	0.62	0.30	0.24	Ala	-1.92	-2.21	1.58	1.38	1.17
Val	0.45	-1.87	1.09	0.11	0.22	Val	-1.90	-1.34	1.31	0.78	1.15
Leu	0.16	-1.72	1.01	-0.11	0.66	Leu	-1.92	-1.82	1.57	0.66	1.51
Ile	0.37	-2.05	1.08	0.32	0.29	Ile	-1.80	-0.90	1.36	1.18	0.16
Met	0.18	-1.99	0.80	0.34	0.67	Met	-1.77	-2.30	1.62	1.26	1.19
Phe	0.83	-1.95	0.49	0.00	0.63	Phe	-0.87	-1.45	0.22	-0.11	2.21
Tyr	1.05	-1.66	0.13	-0.40	0.87	Tyr	-0.66	-1.22	-0.24	-0.52	2.63
His	0.60	-1.85	0.29	0.22	0.74	His	-0.98	-1.33	-0.30	0.33	2.28
Trp	0.80	-1.91	0.26	0.18	0.68	Trp	-1.84	-1.70	1.81	-0.25	1.98
Cys	-0.06	-2.54	2.55	-0.20	0.25	Cys	-2.29	-2.92	3.29	0.78	1.14
Ser	0.32	-1.89	0.96	0.03	0.59	Ser	-1.91	-1.97	1.87	1.04	0.97
Thr	0.22	-2.68	1.44	0.43	0.59	Thr	-1.70	-3.19	2.21	1.44	1.24
Asn	0.40	-2.01	0.11	0.80	0.70	Asn	-1.42	-1.98	0.85	1.00	1.55
Gln	0.11	-1.39	0.61	-0.29	0.97	Gln	-1.99	-2.19	1.90	1.04	1.24
Asp	0.32	-1.10	-0.74	0.05	1.48	Asp	-1.70	-0.34	0.19	-0.42	2.27
Glu	0.58	-1.47	-0.10	0.07	0.91	Glu	-1.94	-1.39	0.63	0.96	1.75
Lys	0.15	-1.59	1.07	0.01	0.36	Lys	-1.67	-0.77	0.39	0.95	1.11
Arg	0.65	-1.43	0.77	-0.26	0.27	Arg	-0.74	-1.38	0.17	0.23	1.71

PBE/cc-pVTZ//PBE/6-31G**						PBE-D[a]/cc-pVTZ//PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	3.34	3.24	-3.13	-2.37	-1.09	Pro	-0.16	0.69	-0.71	1.61	-1.43
Gly	3.53	3.52	-3.22	-3.40	-0.43	Gly	1.29	2.48	-2.31	-2.14	0.67
Ala	3.44	3.48	-3.44	-3.03	-0.45	Ala	1.16	2.78	-2.47	-1.95	0.48
Val	3.37	3.13	-3.16	-2.59	-0.75	Val	1.01	3.67	-2.94	-1.93	0.19
Leu	3.47	3.11	-3.13	-2.78	-0.66	Leu	1.39	3.01	-2.57	-2.01	0.18
Ile	3.16	3.22	-3.22	-2.63	-0.53	Ile	1.00	4.37	-2.94	-1.77	-0.66
Met	2.91	3.45	-3.40	-2.91	-0.04	Met	0.95	3.15	-2.58	-1.99	0.47
Phe	3.31	3.15	-2.57	-2.44	-1.44	Phe	1.60	3.64	-2.83	-2.56	0.14
Tyr	3.16	3.10	-2.37	-2.46	-1.43	Tyr	1.45	3.54	-2.74	-2.58	0.33
His	3.57	3.03	-2.58	-2.76	-1.26	His	2.00	3.55	-3.17	-2.65	0.27
Trp	3.92	3.22	-3.35	-2.63	-1.17	Trp	1.28	3.43	-1.80	-3.06	0.14
Cys	3.09	3.42	-3.04	-2.75	-0.72	Cys	0.86	3.04	-2.29	-1.77	0.16
Ser	3.25	3.45	-3.27	-2.94	-0.49	Ser	1.02	3.37	-2.35	-1.93	-0.11
Thr	3.50	3.22	-3.24	-2.86	-0.62	Thr	1.57	2.71	-2.46	-1.84	0.02
Asn	2.97	3.65	-2.97	-2.67	-0.98	Asn	1.15	3.68	-2.23	-2.48	-0.12
Gln	2.70	3.63	-3.56	-3.15	0.37	Gln	0.61	2.83	-2.27	-1.82	0.65
Asp	1.85	1.38	-1.28	-0.35	-1.60	Asp	-0.16	2.15	-0.36	-0.82	-0.81
Glu	3.26	2.29	-1.83	-2.86	-0.86	Glu	0.74	2.37	-1.11	-1.97	-0.03
Lys	3.65	2.82	-3.24	-2.66	-0.58	Lys	1.84	3.64	-3.92	-1.72	0.17
Arg	2.41	3.28	-3.33	-1.53	-0.83	Arg	1.02	3.33	-3.92	-1.04	0.61

[a] AMBER99 dispersion correction.

PBE/6-31G**// PBE/6-31G**						PBE-D[a]/6-31G**// PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	2.18	1.07	-2.48	-1.59	0.83	Pro	-1.32	-1.49	-0.06	2.38	0.49
Gly	2.28	1.55	-1.96	-2.50	0.63	Gly	0.05	0.51	-1.05	-1.24	1.74
Ala	2.36	1.18	-2.11	-1.91	0.49	Ala	0.08	0.48	-1.14	-0.83	1.41
Val	2.35	0.67	-1.60	-1.51	0.08	Val	0.00	1.20	-1.38	-0.84	1.01
Leu	2.19	0.86	-1.60	-1.91	0.46	Leu	0.11	0.77	-1.04	-1.14	1.31
Ile	2.17	0.66	-1.64	-1.52	0.33	Ile	0.01	1.81	-1.36	-0.65	0.20
Met	1.84	1.04	-1.94	-1.80	0.87	Met	-0.12	0.73	-1.12	-0.88	1.38
Phe	2.28	0.85	-1.53	-1.30	-0.30	Phe	0.58	1.34	-1.79	-1.41	1.28
Tyr	2.20	0.85	-1.50	-1.29	-0.26	Tyr	0.49	1.29	-1.87	-1.42	1.50
His	2.40	0.81	-1.49	-1.64	-0.09	His	0.83	1.33	-2.08	-1.53	1.44
Trp	2.67	0.91	-2.13	-1.41	-0.04	Trp	0.04	1.12	-0.58	-1.85	1.27
Cys	2.06	0.94	-1.63	-1.79	0.42	Cys	-0.17	0.56	-0.89	-0.82	1.31
Ser	2.12	1.27	-1.93	-1.89	0.42	Ser	-0.11	1.20	-1.01	-0.88	0.80
Thr	2.35	0.11	-1.34	-1.54	0.42	Thr	0.43	-0.41	-0.56	-0.52	1.06
Asn	2.02	1.26	-1.89	-1.53	0.14	Asn	0.20	1.28	-1.15	-1.33	0.99
Gln	1.60	1.16	-2.18	-2.19	1.60	Gln	-0.50	0.36	-0.89	-0.85	1.87
Asp	1.29	0.05	-1.92	0.42	0.15	Asp	-0.72	0.82	-0.99	-0.05	0.94
Glu	2.70	0.74	-2.24	-1.51	0.30	Glu	0.18	0.82	-1.51	-0.63	1.14
Lys	2.32	0.56	-1.80	-1.66	0.58	Lys	0.50	1.37	-2.48	-0.72	1.32
Arg	1.88	1.08	-1.73	-2.00	0.76	Arg	0.49	1.14	-2.32	-1.51	2.20

[a] AMBER99 dispersion correction.

B3LYP/cc-pVTZ//B3LYP/6-31G**						B3LYP-D[a]/cc-pVTZ//B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	3.99	4.17	-3.20	-2.69	-2.26	Pro	0.49	1.61	-0.78	1.29	-2.60
Gly	4.20	4.34	-3.55	-3.48	-1.51	Gly	1.97	3.30	-2.65	-2.22	-0.41
Ala	4.17	4.52	-3.74	-3.58	-1.37	Ala	1.89	3.82	-2.77	-2.50	-0.45
Val	4.02	4.12	-3.54	-3.04	-1.55	Val	1.66	4.65	-3.32	-2.37	-0.62
Leu	4.22	4.09	-3.46	-3.21	-1.64	Leu	2.14	3.99	-2.89	-2.44	-0.80
Ile	3.85	4.31	-3.60	-3.05	-1.50	Ile	1.68	5.46	-3.32	-2.18	-1.63
Met	3.49	4.63	-3.85	-3.52	-0.75	Met	1.54	4.33	-3.03	-2.60	-0.24
Phe	3.96	4.05	-2.67	-2.83	-2.52	Phe	2.26	4.55	-2.93	-2.94	-0.93
Tyr	3.85	4.03	-2.60	-2.76	-2.53	Tyr	2.14	4.47	-2.97	-2.88	-0.76
His	4.25	3.83	-2.64	-3.11	-2.33	His	2.68	4.36	-3.23	-3.01	-0.79
Trp	4.81	4.10	-3.68	-3.01	-2.21	Trp	2.17	4.31	-2.13	-3.45	-0.91
Cys	3.88	4.27	-3.25	-3.16	-1.73	Cys	1.65	3.89	-2.51	-2.18	-0.85
Ser	4.11	4.26	-3.69	-3.51	-1.17	Ser	1.88	4.18	-2.77	-2.50	-0.79
Thr	4.23	4.34	-3.71	-3.33	-1.52	Thr	2.30	3.82	-2.93	-2.31	-0.88
Asn	3.71	4.50	-3.35	-2.92	-1.94	Asn	1.89	4.53	-2.61	-2.73	-1.09
Gln	3.31	4.79	-3.96	-3.73	-0.41	Gln	1.21	3.99	-2.67	-2.40	-0.14
Asp	1.91	2.38	-1.37	-0.70	-2.21	Asp	-0.11	3.15	-0.45	-1.17	-1.42
Glu	3.54	2.80	-0.95	-3.51	-1.88	Glu	1.01	2.87	-0.22	-2.62	-1.05
Lys	4.41	3.89	-3.54	-3.12	-1.64	Lys	2.59	4.71	-4.23	-2.18	-0.89
Arg	2.90	4.29	-3.74	-1.25	-2.20	Arg	1.51	4.35	-4.33	-0.77	-0.75

[a] AMBER99 dispersion correction.

B3LYP/6-31G**// B3LYP/6-31G**						B3LYP-D[a]/6-31G**// B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	2.78	2.04	-2.54	-1.92	-0.36	Pro	-0.72	-0.52	-0.12	2.05	-0.70
Gly	2.86	2.32	-2.34	-2.47	-0.38	Gly	0.63	1.28	-1.44	-1.20	0.72
Ala	3.03	2.19	-2.44	-2.47	-0.31	Ala	0.75	1.49	-1.48	-1.39	0.62
Val	2.92	1.69	-2.02	-1.97	-0.62	Val	0.57	2.23	-1.80	-1.30	0.31
Leu	2.86	1.85	-1.98	-2.34	-0.39	Leu	0.78	1.75	-1.41	-1.56	0.45
Ile	2.76	1.77	-2.08	-1.97	-0.48	Ile	0.59	2.92	-1.80	-1.10	-0.61
Met	2.38	2.21	-2.42	-2.43	0.26	Met	0.43	1.91	-1.60	-1.51	0.78
Phe	2.81	1.84	-1.65	-1.71	-1.29	Phe	1.10	2.33	-1.91	-1.82	0.30
Tyr	2.68	1.77	-1.43	-1.69	-1.33	Tyr	0.97	2.21	-1.81	-1.81	0.44
His	2.96	1.65	-1.53	-2.03	-1.05	His	1.39	2.17	-2.12	-1.92	0.49
Trp	3.40	1.82	-2.38	-1.86	-0.97	Trp	0.76	2.03	-0.83	-2.30	0.33
Cys	2.80	1.81	-1.87	-2.23	-0.50	Cys	0.56	1.43	-1.13	-1.25	0.39
Ser	2.95	2.09	-2.39	-2.47	-0.17	Ser	0.72	2.01	-1.48	-1.46	0.21
Thr	3.01	1.26	-1.84	-2.01	-0.41	Thr	1.09	0.74	-1.07	-1.00	0.23
Asn	2.72	2.06	-2.33	-1.77	-0.67	Asn	0.90	2.09	-1.59	-1.58	0.18
Gln	2.17	2.30	-2.61	-2.77	0.91	Gln	0.07	1.51	-1.32	-1.44	1.18
Asp	1.40	1.08	-2.00	-0.16	-0.33	Asp	-0.61	1.85	-1.07	-0.63	0.46
Glu	2.75	1.20	-1.29	-2.18	-0.48	Glu	0.23	1.28	-0.57	-1.29	0.35
Lys	2.99	1.65	-2.13	-2.12	-0.39	Lys	1.17	2.47	-2.81	-1.18	0.35
Arg	2.27	2.13	-2.16	-1.69	-0.56	Arg	0.88	2.19	-2.75	-1.20	0.88

[a] AMBER99 dispersion correction.

	AM1// AM1					AM1-D[a]// AM1					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	2.43	3.50	-3.77	-1.27	-0.88	Pro	-1.07	0.94	-1.35	2.70	-1.22
Gly	2.75	4.57	-3.73	-1.65	-1.95	Gly	0.52	3.54	-2.82	-0.38	-0.85
Ala	2.07	5.18	-3.70	-1.18	-2.36	Ala	-0.21	4.48	-2.73	-0.10	-1.44
Val	1.65	4.81	-3.19	-0.60	-2.68	Val	-0.70	5.35	-2.97	0.07	-1.75
Leu	2.84	3.96	-3.05	-1.19	-2.56	Leu	0.76	3.87	-2.49	-0.42	-1.72
Ile	1.62	4.94	-2.97	-0.49	-3.11	Ile	-0.54	6.09	-2.68	0.37	-3.24
Met	0.44	5.69	-3.75	-1.20	-1.18	Met	-1.51	5.39	-2.93	-0.28	-0.66
Phe	2.92	4.64	-3.05	-0.70	-3.81	Phe	1.22	5.13	-3.31	-0.81	-2.23
Tyr	2.82	4.48	-2.90	-0.59	-3.81	Tyr	1.11	4.92	-3.27	-0.72	-2.04
His	3.03	4.09	-2.96	-0.82	-3.33	His	1.45	4.61	-3.55	-0.72	-1.80
Trp	3.45	4.31	-3.24	-0.97	-3.55	Trp	0.81	4.52	-1.69	-1.40	-2.24
Cys	1.58	4.42	-2.30	-1.24	-2.46	Cys	-0.65	4.04	-1.56	-0.26	-1.58
Ser	0.74	5.38	-3.69	0.91	-3.34	Ser	-1.49	5.30	-2.77	1.92	-2.96
Thr	1.21	4.66	-3.32	-1.00	-1.55	Thr	-0.72	4.15	-2.54	0.02	-0.90
Asn	0.55	6.65	-2.05	-1.92	-3.22	Asn	-1.27	6.67	-1.31	-1.73	-2.36
Gln	0.35	5.00	-3.88	-1.49	0.01	Gln	-1.74	4.20	-2.59	-0.15	0.28
Asp	0.39	4.91	-0.09	-1.47	-3.75	Asp	-1.62	5.68	0.83	-1.93	-2.96
Glu	2.96	2.88	0.41	-2.70	-3.55	Glu	0.44	2.95	1.13	-1.81	-2.71
Lys	2.30	4.39	-3.34	-0.97	-2.38	Lys	0.49	5.20	-4.02	-0.03	-1.63
Arg	-1.04	3.72	-4.81	5.42	-3.29	Arg	-2.43	3.77	-5.40	5.91	-1.85

[a] AMBER99 dispersion correction.

	PM3// PM3					PM3-D[a]// PM3					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	6.36	8.15	-5.01	-4.87	-4.64	Pro	2.86	5.60	-2.59	-0.89	-4.98
Gly	5.56	7.14	-2.90	-2.53	-7.28	Gly	3.33	6.10	-2.00	-1.26	-6.17
Ala	5.77	8.29	-4.44	-2.39	-7.23	Ala	3.49	7.59	-3.47	-1.31	-6.30
Val	5.82	7.92	-4.37	-2.16	-7.21	Val	3.47	8.45	-4.16	-1.49	-6.28
Leu	7.20	6.81	-4.17	-2.25	-7.58	Leu	5.12	6.71	-3.61	-1.48	-6.74
Ile	5.63	8.18	-4.19	-2.23	-7.38	Ile	3.46	9.33	-3.91	-1.37	-7.51
Met	4.14	9.35	-4.75	-2.82	-5.92	Met	2.19	9.05	-3.93	-1.90	-5.41
Phe	5.93	7.94	-3.03	-2.07	-8.77	Phe	4.23	8.43	-3.30	-2.18	-7.18
Tyr	5.96	7.94	-3.43	-1.85	-8.62	Tyr	4.25	8.38	-3.80	-1.97	-6.85
His	6.11	8.43	-3.94	-2.44	-8.17	His	4.54	8.95	-4.53	-2.33	-6.63
Trp	6.62	7.94	-3.78	-2.37	-8.41	Trp	3.99	8.15	-2.23	-2.80	-7.11
Cys	5.03	7.53	-3.45	-1.95	-7.16	Cys	2.80	7.15	-2.71	-0.97	-6.27
Ser	3.90	7.71	-1.93	-2.89	-6.79	Ser	1.67	7.63	-1.01	-1.88	-6.41
Thr	7.11	8.05	-4.92	-3.56	-6.68	Thr	5.19	7.54	-4.15	-2.54	-6.04
Asn	3.76	9.71	-2.58	-2.89	-7.99	Asn	1.94	9.74	-1.84	-2.70	-7.14
Gln	3.97	8.16	-4.85	-2.79	-4.49	Gln	1.87	7.36	-3.56	-1.45	-4.22
Asp	4.81	8.44	0.05	-5.76	-7.54	Asp	2.80	9.20	0.98	-6.23	-6.75
Glu	6.36	5.16	-0.13	-3.87	-7.52	Glu	3.84	5.23	0.60	-2.98	-6.69
Lys	5.75	8.29	-4.61	-2.30	-7.14	Lys	3.94	9.10	-5.29	-1.36	-6.39
Arg	2.22	8.05	-6.15	3.10	-7.21	Arg	0.82	8.10	-6.74	3.58	-5.77

[a] AMBER99 dispersion correction.

PM3MM// PM3MM						PM3MM-D[a]// PM3MM					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	6.31	8.65	-5.58	-5.19	-4.19	Pro	2.82	6.09	-3.16	-1.21	-4.53
Gly	6.26	8.28	-5.14	-3.28	-6.12	Gly	4.03	7.24	-4.23	-2.01	-5.02
Ala	5.84	9.06	-5.30	-3.12	-6.49	Ala	3.57	8.36	-4.33	-2.04	-5.56
Val	5.74	8.57	-5.09	-2.66	-6.57	Val	3.38	9.11	-4.87	-1.99	-5.63
Leu	7.11	7.58	-5.02	-2.78	-6.88	Leu	5.03	7.48	-4.46	-2.01	-6.04
Ile	5.59	8.78	-4.96	-2.75	-6.66	Ile	3.43	9.93	-4.68	-1.88	-6.79
Met	4.26	9.82	-5.57	-3.43	-5.08	Met	2.30	9.52	-4.75	-2.50	-4.57
Phe	6.12	8.89	-4.53	-2.42	-8.05	Phe	4.41	9.38	-4.80	-2.53	-6.47
Tyr	5.99	8.72	-4.35	-2.29	-8.06	Tyr	4.28	9.16	-4.72	-2.42	-6.30
His	6.06	8.93	-4.53	-2.74	-7.71	His	4.49	9.45	-5.13	-2.63	-6.18
Trp	6.60	8.66	-4.73	-2.62	-7.91	Trp	3.96	8.87	-3.18	-3.06	-6.60
Cys	5.54	8.54	-4.13	-3.62	-6.32	Cys	3.31	8.16	-3.39	-2.65	-5.43
Ser	4.67	9.49	-5.65	-1.20	-7.30	Ser	2.44	9.41	-4.73	-0.19	-6.92
Thr	7.62	9.51	-5.70	-6.15	-5.27	Thr	5.69	8.99	-4.93	-5.14	-4.63
Asn	4.49	10.66	-4.27	-3.54	-7.35	Asn	2.67	10.69	-3.52	-3.34	-6.49
Gln	4.25	9.14	-5.68	-3.77	-3.94	Gln	2.15	8.34	-4.39	-2.44	-3.67
Asp	4.87	5.77	1.26	-4.32	-7.58	Asp	2.86	6.54	2.18	-4.79	-6.79
Glu	5.34	6.73	-0.73	-4.23	-7.11	Glu	2.82	6.80	0.00	-3.34	-6.28
Lys	6.63	9.05	-5.77	-3.30	-6.61	Lys	4.81	9.87	-6.45	-2.36	-5.87
Arg	3.48	8.76	-7.34	2.00	-6.90	Arg	2.09	8.81	-7.93	2.49	-5.45

[a] AMBER99 dispersion correction.

AMOEBA// AMOEBA						AMBEREP// AMBEREP					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-2.74	-3.37	2.86	6.28	-3.04	Pro	-13.08	36.00	-6.23	-6.27	-10.43
Gly	0.29	-0.27	0.56	0.55	-1.13	Gly	-1.03	4.79	-1.66	-2.93	0.83
Ala	0.45	-0.53	0.49	0.66	-1.07	Ala	-2.70	6.50	-1.08	-1.87	-0.85
Val	0.03	-0.96	1.26	1.97	-2.30	Val	-1.91	5.72	-1.04	-1.79	-0.98
Leu	0.12	-0.66	0.22	1.32	-1.01	Leu	-2.66	6.33	-0.57	-2.34	-0.75
Ile	-0.34	-1.43	0.94	1.78	-0.95	Ile	-2.65	7.62	-1.14	-2.07	-1.75
Met	-0.41	-0.15	0.66	0.47	-0.57	Met	-3.43	6.24	-0.98	-1.94	0.10
Phe	-0.27	-0.72	0.48	0.78	-0.26	Phe	-2.88	7.05	-1.19	-1.93	-1.06
Tyr	-0.03	-0.82	0.31	0.61	-0.07	Tyr	-2.55	6.82	-1.44	-2.28	-0.55
His	2.68	-0.26	-0.40	-0.57	-1.45	His	-0.55	4.92	-1.92	-1.43	-1.03
Trp	0.43	-0.89	1.17	0.75	-1.47	Trp	-4.14	7.66	-0.26	-1.96	-1.29
Cys	1.18	-0.70	0.11	0.65	-1.24	Cys	-3.84	6.68	1.45	-1.67	-2.62
Ser	-0.25	-2.02	1.17	0.56	0.54	Ser	-2.69	5.95	-0.67	-2.13	-0.45
Thr	1.88	1.51	-0.27	0.31	-3.44	Thr	-2.56	7.08	-0.43	-1.04	-3.05
Asn	1.89	0.79	0.04	-2.57	-0.15	Asn	-2.93	8.72	-0.40	-4.54	-0.86
Gln	0.06	1.14	-0.54	-0.43	-0.22	Gln	-2.53	6.12	-0.62	-1.52	-1.45
Asp	-0.09	-4.39	5.34	0.27	-1.12	Asp	-1.94	1.89	1.50	-2.28	0.83
Glu	-0.64	-2.12	3.37	1.55	-2.16	Glu	-5.96	7.32	1.86	-2.97	-0.25
Lys	2.08	-1.34	-0.24	1.08	-1.58	Lys	-1.94	7.04	-1.69	-2.13	-1.29
Arg	-0.66	0.29	0.75	0.88	-1.25	Arg	-3.22	6.12	-2.42	1.34	-1.82

AMBERPOL// AMBERPOL						AMBER94// AMBER94					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-4.99	0.88	3.44	3.85	-3.17	Pro	-5.55	0.63	1.71	5.23	-2.01
Gly	-1.28	4.29	-0.41	-0.68	-1.91	Gly	-2.86	3.40	0.24	0.57	-1.35
Ala	-2.91	5.95	-0.03	-0.38	-2.63	Ala	-4.49	5.64	0.46	0.78	-2.39
Val	-2.00	4.90	-0.15	-0.35	-2.41	Val	-3.70	4.79	0.28	0.61	-1.98
Leu	-2.83	5.72	0.38	-1.01	-2.27	Leu	-4.57	5.33	-0.40	1.20	-1.56
Ile	-2.90	6.92	-0.12	-0.57	-3.33	Ile	-3.37	5.30	0.53	0.98	-3.44
Met	-3.81	6.38	-0.23	-0.67	-1.68	Met	-4.75	4.62	0.61	0.55	-1.03
Phe	-2.95	6.37	-0.35	-0.63	-2.45	Phe	-4.62	6.09	0.10	0.55	-2.13
Tyr	-2.85	6.59	-0.59	-0.73	-2.42	Tyr	-4.21	5.65	-0.04	0.58	-1.98
His	-1.37	5.28	-0.97	-0.52	-2.41	His	-4.40	5.01	0.13	1.34	-2.08
Trp	-4.18	6.71	0.81	-0.62	-2.71	Trp	-4.85	5.35	1.21	0.53	-2.24
Cys	-3.05	5.88	1.45	-1.07	-3.21	Cys	-4.65	3.84	2.81	0.83	-2.84
Ser	-2.50	5.21	0.11	-0.90	-1.93	Ser	-3.69	2.68	1.85	1.55	-2.38
Thr	-3.76	8.24	-0.46	-0.55	-3.46	Thr	-4.57	5.58	-0.36	0.23	-0.88
Asn	-2.07	7.58	-0.01	-3.38	-2.11	Asn	-2.93	4.47	-0.85	0.83	-1.51
Gln	-2.56	5.56	0.19	-0.21	-2.99	Gln	-5.07	6.51	0.64	0.66	-2.74
Asp	-1.35	1.04	2.20	-1.22	-0.68	Asp	-5.04	1.59	2.80	0.46	0.18
Glu	-5.69	6.47	2.66	-1.48	-1.97	Glu	-7.30	5.21	3.92	-0.84	-0.99
Lys	-2.25	6.50	-1.32	-0.53	-2.41	Lys	-3.90	4.94	0.48	1.49	-3.01
Arg	-3.92	6.17	-1.68	2.37	-2.94	Arg	-5.40	4.88	-0.42	4.91	-3.98

AMBER96// AMBER96						AMBER99// AMBER99					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-0.69	5.49	-1.98	0.12	-2.94	Pro	-3.87	0.27	2.19	2.03	-0.62
Gly	2.01	8.27	-3.45	-4.54	-2.28	Gly	-1.48	2.78	1.19	-2.45	-0.05
Ala	0.37	10.51	-3.23	-4.33	-3.32	Ala	-2.64	4.51	1.14	-2.19	-0.81
Val	1.17	9.66	-3.41	-4.50	-2.91	Val	-1.83	3.63	0.96	-2.36	-0.40
Leu	0.29	10.20	-4.09	-3.91	-2.49	Leu	-2.74	4.19	0.25	-1.71	0.01
Ile	1.50	10.17	-3.16	-4.13	-4.37	Ile	-1.44	4.03	1.22	-1.97	-1.84
Met	0.12	9.49	-3.08	-4.56	-1.96	Met	-2.89	3.49	1.28	-2.43	0.55
Phe	0.25	10.96	-3.59	-4.56	-3.06	Phe	-2.76	4.97	0.78	-2.43	-0.56
Tyr	0.66	10.52	-3.73	-4.53	-2.91	Tyr	-2.35	4.53	0.63	-2.39	-0.41
His	0.46	9.88	-3.57	-3.77	-3.01	His	-2.55	3.88	0.80	-1.62	-0.51
Trp	0.02	10.22	-2.48	-4.59	-3.17	Trp	-2.99	4.24	1.88	-2.45	-0.67
Cys	0.22	8.70	-0.88	-4.28	-3.76	Cys	-2.80	2.70	3.49	-2.13	-1.26
Ser	1.18	7.54	-1.85	-3.56	-3.31	Ser	-1.85	1.52	2.53	-1.41	-0.79
Thr	0.30	10.45	-4.05	-4.89	-1.80	Thr	-2.68	4.35	0.34	-2.73	0.72
Asn	1.93	9.34	-4.55	-4.28	-2.44	Asn	-1.23	3.17	-0.34	-1.53	-0.07
Gln	-0.20	11.38	-3.06	-4.45	-3.66	Gln	-3.49	5.80	1.05	-2.58	-0.78
Asp	-0.17	6.46	-0.89	-4.65	-0.74	Asp	-3.19	0.30	3.67	-2.51	1.74
Glu	-2.44	10.08	0.23	-5.95	-1.92	Glu	-5.53	4.37	4.52	-3.88	0.52
Lys	0.97	9.80	-3.22	-3.62	-3.94	Lys	-2.04	3.85	1.14	-1.50	-1.45
Arg	-0.53	9.75	-4.11	-0.20	-4.90	Arg	-3.59	3.79	0.19	2.08	-2.47

AMBER99SB// AMBER99SB						AMBER03// AMBER03					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	1.16	1.70	1.12	0.37	-4.35	Pro	-1.56	6.10	1.69	-1.09	-5.14
Gly	2.78	2.81	-0.18	-1.93	-3.47	Gly	0.32	7.16	-1.39	-2.33	-3.76
Ala	2.67	3.52	-0.39	-2.13	-3.67	Ala	-0.74	10.58	-1.74	-3.18	-4.92
Val	3.49	2.65	-0.56	-2.29	-3.29	Val	1.08	7.98	-2.04	-3.58	-3.44
Leu	2.55	3.23	-1.28	-1.65	-2.84	Leu	-0.80	10.34	-2.28	-2.56	-4.70
Ile	3.90	3.08	-0.26	-1.87	-4.84	Ile	1.41	12.02	-2.92	-4.27	-6.24
Met	2.41	2.50	-0.26	-2.36	-2.28	Met	-1.25	8.28	-0.76	-2.55	-3.72
Phe	2.53	3.98	-0.76	-2.36	-3.39	Phe	-1.17	9.18	-1.29	-2.48	-4.24
Tyr	2.93	3.53	-0.89	-2.30	-3.27	Tyr	-3.43	8.87	-0.46	-1.46	-3.51
His	2.78	2.90	-0.71	-1.53	-3.44	His	-3.75	7.66	0.09	-0.42	-3.59
Trp	2.30	3.26	0.33	-2.35	-3.54	Trp	-3.04	7.91	-0.35	-1.51	-3.01
Cys	2.52	1.74	1.81	-2.04	-4.03	Cys	-1.04	8.25	0.84	-2.74	-5.32
Ser	3.47	0.57	0.98	-1.38	-3.65	Ser	-0.52	9.44	-0.96	-3.19	-4.78
Thr	3.28	3.13	-1.13	-2.62	-2.66	Thr	0.93	11.62	-2.77	-3.04	-6.75
Asn	3.92	2.24	-1.92	-1.26	-2.97	Asn	-0.08	6.95	-2.28	-1.33	-3.27
Gln	1.51	5.38	-0.76	-2.82	-3.31	Gln	0.02	14.78	-3.43	-5.54	-5.83
Asp	2.05	-0.72	2.20	-2.41	-1.13	Asp	-2.60	6.67	1.44	-4.05	-1.46
Glu	-0.17	3.24	3.06	-3.77	-2.35	Glu	-1.02	10.81	1.28	-6.53	-4.54
Lys	3.26	2.91	-0.39	-1.45	-4.34	Lys	3.96	6.19	-1.82	-1.79	-6.54
Arg	1.70	2.83	-1.35	2.20	-5.38	Arg	-1.05	5.63	-2.26	4.64	-6.96

CHARMM27// CHARMM27						OPLS-AA// OPLS-AA					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-1.96	9.14	-1.01	0.05	-6.23	Pro	-0.62	0.23	-1.34	6.55	-4.81
Gly	0.18	11.84	-4.69	-3.77	-3.57	Gly	2.31	4.38	-2.55	-2.47	-1.66
Ala	-2.52	15.53	-4.20	-2.86	-5.95	Ala	2.02	5.62	-3.02	-2.18	-2.45
Val	-2.46	15.67	-4.54	-2.59	-6.07	Val	2.30	5.29	-2.84	-1.86	-2.89
Leu	-1.88	14.74	-4.57	-2.25	-6.04	Leu	2.71	4.91	-3.28	-1.87	-2.47
Ile	-2.36	16.06	-4.41	-2.39	-6.90	Ile	2.63	6.02	-2.56	-1.46	-4.63
Met	-2.83	15.70	-4.35	-3.33	-5.19	Met	1.04	6.36	-4.09	-3.62	0.31
Phe	-1.12	15.03	-4.50	-2.93	-6.48	Phe	3.54	4.26	-3.11	-1.78	-2.92
Tyr	-0.99	14.93	-4.61	-2.97	-6.37	Tyr	3.65	4.15	-3.18	-1.80	-2.82
His	0.05	11.91	-3.79	-1.98	-6.19	His	3.14	3.86	-2.85	-1.51	-2.64
Trp	-1.74	14.66	-4.18	-2.89	-5.85	Trp	1.26	5.92	-4.17	-1.12	-1.89
Cys	-2.26	14.41	-2.47	-2.95	-6.73	Cys	2.79	4.05	-1.89	-2.60	-2.34
Ser	-2.16	12.74	-3.89	-3.17	-3.52	Ser	2.84	3.73	-2.77	-2.47	-1.34
Thr	-2.53	16.46	-5.36	-3.23	-5.34	Thr	3.11	4.29	-2.46	-1.22	-3.72
Asn	-2.11	15.45	-2.63	-4.28	-6.43	Asn	4.38	2.90	-5.77	-0.79	-0.72
Gln	-3.17	16.67	-4.47	-3.38	-5.65	Gln	1.81	4.68	-1.38	-0.96	-4.15
Asp	-7.76	13.61	3.22	-2.83	-6.24	Asp	0.71	-1.22	-2.48	2.74	0.25
Glu	-6.48	15.06	0.21	-3.03	-5.77	Glu	-0.38	4.13	2.22	-3.10	-2.88
Lys	-1.06	14.61	-4.70	-2.50	-6.35	Lys	4.19	5.28	-3.89	-2.41	-3.18
Arg	-2.44	14.59	-5.67	1.44	-7.93	Arg	1.23	5.43	-4.57	2.70	-4.79

OPLS-AA/L// OPLS-AA/L					
	α_R	α_L	β	β_a	PPII
Pro	-0.91	0.87	-0.50	6.99	-6.44
Gly	4.62	7.54	-5.25	-5.18	-1.74
Ala	1.59	6.50	-1.87	-2.51	-3.71
Val	1.77	6.05	-1.74	-2.27	-3.80
Leu	2.45	5.55	-1.87	-2.17	-3.96
Ile	1.45	6.33	-2.09	-2.48	-3.21
Met	0.63	7.30	-3.04	-3.96	-0.93
Phe	3.08	5.09	-1.99	-1.90	-4.28
Tyr	3.19	4.95	-2.10	-1.87	-4.16
His	2.90	4.06	-1.74	-1.50	-3.71
Trp	1.25	6.27	-2.67	-1.51	-3.33
Cys	2.86	5.54	-1.51	-3.79	-3.09
Ser	3.17	5.47	-0.82	-2.33	-5.49
Thr	2.36	5.40	-1.55	-1.57	-4.65
Asn	3.19	5.77	-2.11	-3.78	-3.07
Gln	1.77	6.22	-1.67	-2.19	-4.14
Asp	-2.33	1.48	2.00	1.10	-2.26
Glu	-3.13	6.62	1.20	-1.96	-2.74
Lys	3.11	6.18	-2.62	-2.47	-4.21
Arg	1.15	6.00	-3.38	2.27	-6.04

AMBERUA// AMBERUA					
	α_R	α_L	β	β_a	PPII
Pro	-10.27	42.71	-9.13	-8.37	-14.95
Gly	0.04	9.11	-1.97	-3.11	-4.07
Ala	-2.67	11.72	-1.38	-2.87	-4.81
Val	-0.32	8.02	-0.59	-1.92	-5.20
Leu	-2.93	11.43	-1.57	-2.54	-4.39
Ile	-1.91	9.72	-0.76	-2.10	-4.95
Met	-2.53	9.68	-1.04	-2.47	-3.63
Phe	-2.47	11.41	-1.33	-2.73	-4.87
Tyr	-5.36	11.05	-0.39	-1.61	-3.70
His	-3.01	10.57	-0.98	-1.91	-4.67
Trp	-3.71	10.57	-0.29	-2.14	-4.43
Cys	-3.00	10.08	0.81	-2.65	-5.23
Ser	-3.25	8.65	-0.64	-2.59	-2.17
Thr	-2.16	13.56	-3.30	-4.49	-3.60
Asn	-0.60	9.82	-2.85	-2.17	-4.20
Gln	-2.02	12.82	-1.38	-3.27	-6.14
Asp	-3.22	8.65	0.31	-2.74	-3.00
Glu	-2.82	10.04	1.86	-4.75	-4.33
Lys	-2.10	9.20	-0.94	-1.61	-4.54
Arg	-2.10	7.43	-2.42	3.41	-6.32

GROMOS(G43b1)// GROMOS(G43b1)					
	α_R	α_L	β	β_a	PPII
Pro	-6.63	35.92	-10.21	-6.88	-12.19
Gly	3.81	6.39	-5.16	-2.88	-2.16
Ala	3.26	7.49	-5.45	-2.72	-2.58
Val	3.56	6.18	-4.81	-1.74	-3.20
Leu	3.85	6.41	-5.22	-2.70	-2.34
Ile	3.28	6.75	-4.97	-1.85	-3.21
Met	2.44	8.40	-5.68	-2.95	-2.20
Phe	2.96	8.45	-5.56	-3.38	-2.47
Tyr	3.03	8.39	-5.55	-3.89	-1.99
His	2.93	7.99	-4.83	-2.73	-3.36
Trp	1.40	8.49	-3.83	-3.07	-2.99
Cys	3.18	7.99	-4.01	-3.18	-3.97
Ser	2.40	7.15	-4.90	-2.66	-1.99
Thr	3.73	5.88	-4.76	-2.43	-2.42
Asn	3.39	8.63	-4.34	-4.48	-3.20
Gln	2.48	7.75	-4.77	-2.15	-3.31
Asp	11.79	-5.59	4.51	-2.04	-8.68
Glu	2.98	3.67	6.07	-5.00	-7.72
Lys	3.99	6.00	-6.48	-2.56	-0.96
Arg	-4.64	6.52	-7.90	8.65	-2.62

GROMOS(G45a3)// GROMOS(G45a3)					
	α_R	α_L	β	β_a	PPII
Pro	-5.60	34.73	-10.28	-7.05	-11.79
Gly	4.34	5.24	-5.07	-2.77	-1.74
Ala	4.00	5.70	-5.28	-2.53	-1.89
Val	3.86	5.61	-4.92	-1.68	-2.86
Leu	4.44	4.60	-5.36	-2.10	-1.58
Ile	3.51	5.63	-5.08	-1.68	-2.37
Met	2.88	7.21	-5.68	-2.84	-1.57
Phe	3.69	7.07	-5.54	-3.24	-1.98
Tyr	3.64	6.98	-5.59	-3.52	-1.51
His	3.45	6.44	-4.89	-1.99	-3.01
Trp	2.07	7.07	-3.65	-2.87	-2.62
Cys	3.77	6.60	-3.94	-3.00	-3.43
Ser	2.98	5.73	-4.82	-2.50	-1.40
Thr	4.00	5.28	-5.02	-2.44	-1.81
Asn	3.97	7.26	-4.21	-4.35	-2.68
Gln	2.86	6.59	-4.95	-2.13	-2.36
Asp	3.44	4.00	4.80	-4.71	-7.53
Glu	1.14	3.87	7.31	-5.39	-6.94
Lys	4.19	3.59	-6.00	-1.43	-0.36
Arg	-0.12	2.80	-7.51	7.27	-2.44

GROMOS(G53a6)// GROMOS(G53a6)					
	α_R	α_L	β	β_a	PPII
Pro	-8.27	34.26	-12.74	2.84	-16.09
Gly	5.97	6.78	-6.27	-4.45	-2.03
Ala	5.62	7.32	-6.49	-4.20	-2.26
Val	5.33	7.37	-6.32	-3.29	-3.09
Leu	6.40	6.29	-6.43	-3.41	-2.84
Ile	5.06	7.51	-6.39	-3.19	-2.99
Met	4.13	6.28	-5.88	-3.55	-0.99
Phe	5.56	8.02	-6.63	-4.40	-2.55
Tyr	5.49	7.99	-6.69	-4.72	-2.07
His	4.89	7.61	-6.85	-3.02	-2.63
Trp	3.97	8.21	-4.87	-3.85	-3.46
Cys	5.54	6.36	-4.57	-4.45	-2.88
Ser	4.89	6.56	-5.18	-3.50	-2.77
Thr	5.28	7.55	-5.65	-3.07	-4.11
Asn	5.06	8.33	-6.05	-3.96	-3.37
Gln	4.10	9.58	-5.98	-3.69	-4.01
Asp	3.04	6.95	2.10	-5.61	-6.48
Glu	2.90	5.11	3.92	-6.31	-5.62
Lys	5.58	5.59	-6.75	-2.92	-1.50
Arg	2.44	4.75	-8.39	4.71	-3.51

Table S3c. Signed RMS-C (kcal/mol) of each conformation over 20 amino acids for each method.

	α_R	α_L	β	β_a	PPII	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.22	0.62	-0.52	-0.79	-0.78	0.79	0.24
M05-2X-D[a]/cc-pVTZ	-1.09	0.86	0.92	0.89	0.54	0.86	0.18
M05-2X/6-31G**	0.48	-1.79	0.93	0.31	0.70	0.84	0.52
M05-2X-D[a]/6-31G**	-1.81	-1.97	1.54	1.24	1.59	1.63	0.25
PBE/cc-pVTZ	3.22	3.18	-3.02	-2.66	-0.91	2.60	0.87
PBE-D[a]/cc-pVTZ	1.21	3.16	-2.55	-2.05	0.51	1.90	0.94
PBE/6-31G**	2.19	0.95	-1.85	-1.69	0.58	1.45	0.60
PBE-D[a]/6-31G**	0.48	1.08	-1.39	-1.19	1.31	1.09	0.32
B3LYP/cc-pVTZ	3.89	4.12	-3.30	-3.06	-1.83	3.24	0.80
B3LYP-D[a]/cc-pVTZ	1.85	4.09	-2.83	-2.42	-1.04	2.45	1.02
B3LYP/6-31G**	2.75	1.87	-2.11	-2.08	-0.68	1.90	0.68
B3LYP-D[a]/6-31G**	0.81	1.91	-1.63	-1.50	0.56	1.28	0.51
AM1	2.11	4.68	-3.20	-1.74	-2.83	2.91	1.02
AM1-D[a]	-1.17	4.70	-2.81	1.74	-1.98	2.48	1.23
PM3	5.54	8.01	-3.93	-3.01	-7.27	5.55	1.90
PM3-D[a]	3.48	7.99	-3.54	-2.44	-6.39	4.77	2.08
PM3MM	5.73	8.74	-4.98	-3.45	-6.71	5.92	1.77
PM3MM-D[a]	3.67	8.69	-4.56	-2.76	-5.83	5.10	2.06
AMOEBA	1.21	-1.61	1.67	1.78	-1.54	1.56	0.19
AMBEREP	-4.11	10.24	-1.89	-2.59	-2.68	4.30	3.06
AMBERPOL	-3.17	5.91	1.29	-1.45	-2.54	2.87	1.67
AMBER94	-4.60	4.80	1.45	1.81	-2.22	2.98	1.43
AMBER96	1.04	9.55	-3.15	-4.20	-3.09	4.21	2.86
AMBER99	-2.86	3.78	1.90	-2.28	-1.02	2.37	0.93
AMBER99SB	2.72	2.98	-1.25	-2.16	-3.53	2.53	0.78
AMBER03	-1.89	9.11	-1.83	-3.28	-4.79	4.18	2.69
CHARMM27	-2.99	14.55	-4.10	-2.87	-6.02	6.11	4.37
OPLS-AA	2.60	4.58	-3.20	-2.57	-2.96	3.18	0.74
OPLS-AA/L	2.54	5.70	-2.31	-3.02	-3.97	3.51	1.23
AMBERUA	-3.50	13.86	-2.54	-3.32	-5.54	5.75	4.17
GROMOS(G43b1)	4.33	10.65	-5.63	-3.79	-4.53	5.79	2.50
GROMOS(G45a3)	3.59	9.60	-5.68	-3.66	-4.05	5.32	2.27
GROMOS(G53a6)	5.14	10.36	-6.51	-4.06	-4.87	6.19	2.23

[1] Standard deviation. [a] AMBER99 dispersion correction.

Table S3d. RMS(kcal/mol) over the five conformations of the tetrapeptides.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	0.93	1.00	0.83	0.82	0.76	0.75	0.65	0.89	0.97	0.80	1.04	0.94	0.70	0.64	0.68	0.87	0.42	0.79	0.83	0.90	0.81	0.14
M05-2X-D[a]/cc-pVTZ	2.21	0.52	0.55	0.77	0.51	0.98	0.47	0.66	0.91	0.68	0.79	1.16	0.58	0.49	0.35	0.62	1.07	0.99	0.84	0.62	0.79	0.39
M05-2X/6-31G**	0.60	0.68	0.77	1.00	0.94	1.07	1.02	1.01	0.98	0.94	0.98	1.62	0.99	1.40	1.03	0.82	0.90	0.82	0.88	0.80	0.96	0.22
M05-2X-D[a]/6-31G**	3.02	1.66	1.69	1.35	1.56	1.21	1.68	1.25	1.35	1.27	1.65	2.30	1.62	2.08	1.42	1.73	1.29	1.42	1.06	1.05	1.58	0.45
PBE/cc-pVTZ	2.77	3.06	3.00	2.77	2.82	2.76	2.84	2.66	2.58	2.75	3.01	2.78	2.90	2.89	2.79	2.94	1.39	2.37	2.80	2.48	2.72	0.35
PBE-D[a]/cc-pVTZ	1.06	1.91	1.96	2.32	2.08	2.54	2.08	2.47	2.40	2.60	2.28	1.92	2.08	1.96	2.28	1.86	1.10	1.50	2.64	2.41	2.07	0.43
PBE/6-31G**	1.75	1.90	1.75	1.47	1.55	1.43	1.56	1.42	1.38	1.50	1.70	1.50	1.65	1.41	1.52	1.79	1.05	1.75	1.55	1.57	1.56	0.18
PBE-D[a]/6-31G**	1.40	1.09	0.92	1.01	0.97	1.06	0.95	1.34	1.39	1.50	1.15	0.84	0.88	0.64	1.07	1.04	0.78	0.97	1.45	1.68	1.11	0.26
B3LYP/cc-pVTZ	3.34	3.56	3.65	3.38	3.45	3.40	3.50	3.27	3.22	3.31	3.67	3.37	3.53	3.57	3.39	3.57	1.82	2.72	3.45	3.07	3.31	0.40
B3LYP-D[a]/cc-pVTZ	1.54	2.32	2.54	2.88	2.66	3.20	2.72	2.96	2.91	3.04	2.85	2.43	2.67	2.63	2.81	2.46	1.64	1.86	3.23	2.87	2.61	0.46
B3LYP/6-31G**	2.10	2.25	2.29	1.99	2.05	1.96	2.12	1.93	1.84	1.95	2.23	1.99	2.23	1.91	2.03	2.25	1.21	1.77	2.04	1.87	2.00	0.23
B3LYP-D[a]/6-31G**	1.05	1.10	1.21	1.44	1.29	1.65	1.36	1.66	1.59	1.74	1.47	1.03	1.34	0.89	1.43	1.22	1.05	0.87	1.84	1.75	1.35	0.29
AM1	2.64	3.13	3.22	2.95	2.86	3.03	3.15	3.30	3.20	3.04	3.30	2.64	3.32	2.74	3.54	2.91	2.85	2.72	2.91	3.96	3.07	0.31
AM1-D[a]	1.59	2.08	2.43	2.86	2.23	3.32	2.84	2.98	2.86	2.82	2.49	2.08	3.18	2.24	3.36	2.34	3.10	2.04	3.04	4.19	2.70	0.58
PM3	5.95	5.47	6.00	5.87	5.97	5.93	5.83	6.14	6.13	6.27	6.29	5.46	5.15	6.28	6.12	5.17	6.07	5.27	5.99	5.82	5.86	0.35
PM3-D[a]	3.79	4.29	4.97	5.34	5.14	5.87	5.20	5.59	5.54	5.84	5.40	4.61	4.62	5.36	5.66	4.25	5.96	4.38	5.81	5.62	5.16	0.62
PM3MM	6.17	6.04	6.26	6.04	6.14	6.08	6.05	6.44	6.34	6.39	6.49	5.89	6.30	7.02	6.61	5.72	5.19	5.34	6.54	6.23	6.16	0.41
PM3MM-D[a]	3.93	4.81	5.22	5.55	5.32	6.03	5.40	5.98	5.83	6.01	5.61	5.01	5.74	6.09	6.12	4.75	4.99	4.58	6.36	6.01	5.47	0.62
AMOEBA	3.89	0.64	0.68	1.53	0.81	1.19	0.48	0.55	0.48	1.40	1.01	0.88	1.11	1.89	1.47	0.60	3.13	2.16	1.40	0.83	1.31	0.87
AMBEREP	18.19	2.68	3.31	2.89	3.27	3.84	3.33	3.59	3.48	2.50	4.04	3.77	3.09	3.67	4.61	3.12	1.76	4.51	3.53	3.43	4.13	3.29
AMBERPOL	3.53	2.21	3.19	2.61	3.07	3.68	3.42	3.34	3.41	2.71	3.76	3.39	2.76	4.35	3.94	3.05	1.39	4.18	3.32	3.76	3.25	0.67
AMBER94	3.62	2.10	3.42	2.86	3.27	3.24	3.02	3.56	3.28	3.18	3.43	3.25	2.54	3.25	2.54	3.91	2.69	4.42	3.20	4.31	3.25	0.55
AMBER96	2.94	4.69	5.49	5.20	5.34	5.51	4.98	5.71	5.55	5.17	5.32	4.67	4.13	5.53	5.21	5.87	3.60	5.41	5.22	5.22	5.04	0.71
AMBER99	2.21	1.86	2.61	2.15	2.37	2.33	2.38	2.80	2.54	2.24	2.72	2.59	1.72	2.62	1.67	3.29	2.57	4.13	2.22	2.75	2.49	0.53
AMBER99SB	2.21	2.51	2.74	2.67	2.43	3.22	2.14	2.82	2.75	2.48	2.61	2.57	2.39	2.67	2.62	3.18	1.82	2.81	2.83	3.05	2.63	0.33
AMBER03	3.75	3.82	5.47	4.33	5.32	6.52	4.27	4.72	4.58	4.14	4.08	4.60	4.97	6.30	3.63	7.68	3.79	6.05	4.55	4.64	4.86	1.04
CHARMM27	5.05	6.15	7.86	7.95	7.53	8.20	7.89	7.72	7.67	6.30	7.46	7.39	6.40	8.31	7.87	8.38	7.78	7.89	7.53	7.95	7.46	0.82
OPLS-AA	3.69	2.82	3.33	3.26	3.22	3.83	3.78	3.23	3.22	2.90	3.43	2.83	2.74	3.14	3.52	3.01	1.77	2.83	3.91	4.05	3.23	0.51
OPLS-AA/L	4.29	5.21	3.70	3.53	3.48	3.55	3.99	3.50	3.46	2.97	3.50	3.61	3.90	3.50	3.78	3.65	1.90	3.64	3.96	4.25	3.67	0.60
AMBERUA	21.48	4.76	5.96	4.37	5.79	5.05	4.91	5.82	5.78	5.42	5.47	5.40	4.41	6.82	5.04	6.61	4.51	5.54	4.76	4.84	6.14	3.58
GROMOS(G43b1)	18.08	4.36	4.70	4.18	4.38	4.35	4.95	5.07	5.09	4.79	4.63	4.81	4.29	4.07	5.20	4.57	7.35	5.36	4.50	6.45	5.56	2.97
GROMOS(G45a3)	17.50	4.07	4.15	4.04	3.91	3.95	4.54	4.66	4.64	4.25	4.07	4.34	3.83	3.96	4.74	4.15	5.10	5.42	3.70	4.96	5.00	2.90
GROMOS(G53a6)	18.28	5.38	5.48	5.35	5.32	5.33	4.57	5.75	5.75	5.38	5.17	4.90	4.77	5.35	5.63	5.90	5.21	4.92	4.88	5.17	5.92	2.86

[1] Standard deviation. [a] AMBER99 dispersion correction.

Table S4a. Energy offset (E_c) for each tetrapeptide obtained from Eq. 2 in minimizing RMS of each method over 4 conformations (excluding α_L).

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg
M05-2X/cc-pVTZ	1.40	1.58	1.43	1.37	1.30	1.29	1.17	1.66	1.81	1.51	1.99	0.74	1.27	1.13	1.23	1.27	0.51	0.94	1.39	1.32
M05-2X-D[a]/cc-pVTZ	-2.74	-0.91	-1.02	-0.85	-0.81	-0.59	-0.86	0.08	0.21	0.07	-0.60	-1.59	-0.98	-0.92	-0.58	-1.02	-1.31	-1.56	-0.22	-0.05
M05-2X/6-31G**	-0.05	0.06	-0.02	-0.02	-0.27	-0.15	-0.32	0.34	0.64	0.13	0.32	-0.69	-0.15	-0.45	-0.10	-0.24	0.04	0.22	-0.25	0.30
M05-2X-D[a]/6-31G**	-4.19	-2.44	-2.47	-2.24	-2.38	-2.03	-2.35	-1.24	-0.96	-1.31	-2.27	-3.02	-2.40	-2.50	-1.92	-2.53	-1.78	-2.29	-1.86	-1.08
PBE/cc-pVTZ	4.15	4.41	4.31	4.15	4.25	3.97	3.77	4.09	3.93	4.33	4.73	3.94	4.11	4.30	3.88	3.61	2.19	3.83	4.36	3.23
PBE-D[a]/cc-pVTZ	0.01	1.91	1.85	1.93	2.14	2.09	1.74	2.52	2.33	2.88	2.14	1.62	1.86	2.25	2.07	1.31	0.37	1.33	2.74	1.86
PBE/6-31G**	2.45	2.67	2.65	2.52	2.40	2.34	2.10	2.49	2.42	2.61	2.90	2.30	2.44	2.38	2.34	1.89	1.30	2.89	2.46	2.15
PBE-D[a]/6-31G**	-1.69	0.17	0.20	0.30	0.30	0.46	0.07	0.91	0.82	1.16	0.32	-0.03	0.19	0.33	0.52	-0.40	-0.52	0.39	0.85	0.78
B3LYP/cc-pVTZ	5.03	5.29	5.30	5.04	5.24	4.92	4.65	4.98	4.86	5.21	5.83	4.95	5.18	5.31	4.84	4.51	2.50	4.24	5.39	3.97
B3LYP-D[a]/cc-pVTZ	0.89	2.79	2.85	2.82	3.14	3.04	2.62	3.40	3.26	3.77	3.25	2.62	2.93	3.26	3.02	2.21	0.68	1.73	3.77	2.59
B3LYP/6-31G**	3.29	3.44	3.58	3.34	3.32	3.20	2.93	3.27	3.12	3.37	3.85	3.25	3.47	3.33	3.23	2.75	1.67	3.05	3.40	2.81
B3LYP-D[a]/6-31G**	-0.85	0.95	1.13	1.12	1.21	1.32	0.90	1.69	1.52	1.93	1.27	0.92	1.22	1.28	1.42	0.45	-0.15	0.55	1.79	1.43
AM1	3.30	3.90	3.36	2.86	3.83	2.86	1.86	4.08	3.94	4.05	4.53	2.69	2.08	2.37	2.21	1.60	1.62	3.68	3.40	-0.11
AM1-D[a]	-0.84	1.40	0.91	0.64	1.72	0.98	-0.17	2.50	2.34	2.60	1.94	0.36	-0.16	0.32	0.39	-0.69	-0.20	1.18	1.79	-1.49
PM3	8.40	7.34	7.84	7.80	8.90	7.67	6.48	7.91	7.94	8.22	8.61	6.91	5.83	9.13	6.19	6.01	6.92	7.65	7.83	4.23
PM3-D[a]	4.26	4.85	5.39	5.58	6.79	5.79	4.45	6.33	6.34	6.78	6.02	4.58	3.58	7.07	4.37	3.71	5.10	5.15	6.21	2.85
PM3MM	8.48	8.33	8.11	7.88	9.00	7.79	6.71	8.34	8.17	8.29	8.77	7.67	7.04	9.99	7.15	6.53	6.31	7.03	8.89	5.67
PM3MM-D[a]	4.34	5.84	5.66	5.66	6.90	5.91	4.68	6.76	6.57	6.85	6.18	5.35	4.79	7.94	5.34	4.24	4.49	4.52	7.28	4.29
AMOEBA	-3.58	0.22	0.32	-0.21	-0.04	-0.70	-0.45	-0.45	-0.24	2.61	0.21	1.00	-0.76	2.26	2.08	0.34	-1.19	-1.17	1.74	-0.59
AMBEREP	-4.08	0.17	-1.07	-0.48	-1.08	-0.74	-1.87	-1.11	-0.84	0.68	-2.23	-2.17	-1.20	-0.79	-0.75	-1.00	-1.47	-4.13	-0.18	-1.69
AMBERPOL	-4.77	-0.21	-1.42	-0.77	-1.40	-1.17	-2.21	-1.35	-1.20	-0.05	-2.51	-1.58	-1.20	-1.70	-0.18	-1.17	-1.08	-4.07	-0.62	-2.38
AMBER94	-5.40	-2.01	-3.08	-2.50	-3.24	-2.04	-3.59	-3.09	-2.79	-3.15	-3.51	-3.69	-3.02	-3.18	-1.82	-3.44	-4.64	-6.00	-2.66	-4.18
AMBER96	0.68	4.08	3.00	3.58	2.84	4.04	2.49	2.99	3.29	2.93	2.57	2.39	3.06	2.91	4.27	2.64	1.44	0.08	3.42	1.91
AMBER99	-3.81	-0.78	-1.52	-0.93	-1.70	-0.44	-2.02	-1.52	-1.22	-1.58	-1.93	-2.12	-1.47	-1.60	-0.43	-2.04	-3.12	-4.43	-1.07	-2.64
AMBER99SB	1.59	3.48	3.55	4.15	3.36	4.67	3.03	3.52	3.82	3.51	3.12	2.95	3.62	4.06	4.47	2.86	1.87	0.64	3.99	2.41
AMBER03	-0.03	2.11	1.91	3.07	1.79	4.41	0.82	1.12	-1.21	-1.83	-1.06	1.03	1.85	3.84	1.66	3.71	-0.93	1.68	5.51	0.35
CHARMM27	0.33	3.15	1.37	1.46	1.81	1.66	1.10	2.64	2.75	3.03	1.92	1.34	1.02	1.58	1.76	1.00	-4.36	-2.72	2.60	1.21
OPLS-AA	-0.57	3.40	3.43	3.62	3.93	4.14	2.63	4.61	4.68	4.10	2.74	3.80	3.78	4.18	5.11	2.98	0.41	0.65	5.51	2.59
OPLS-AA/L	-0.69	6.51	3.22	3.28	3.84	3.04	2.45	4.36	4.42	3.92	2.81	4.25	4.54	3.71	4.63	3.33	-1.96	-1.47	4.66	2.65
AMBERUA	0.41	2.32	0.26	1.69	-0.07	0.52	-0.11	0.38	-2.60	-0.37	-1.07	-0.48	-1.09	1.23	1.85	1.19	-1.06	-0.31	0.20	-0.24
GROMOS(G43b1)	2.35	5.41	5.13	5.11	5.45	4.96	4.54	5.07	5.13	4.93	3.52	5.17	4.19	5.20	5.55	4.41	10.40	3.89	5.49	-3.01
GROMOS(G45a3)	3.08	5.65	5.42	5.26	5.59	4.91	4.68	5.46	5.38	5.06	3.84	5.42	4.42	5.32	5.79	4.50	4.44	2.11	5.09	0.58
GROMOS(G53a6)	0.30	7.67	7.45	7.18	7.97	6.93	5.70	7.56	7.49	6.79	6.03	7.13	6.53	7.17	7.14	6.50	4.78	4.17	6.98	3.63

[a] AMBER99 dispersion correction.

Table S4b. Signed error (*error*=E_{ai}-E_{bi}+E_c, kcal/mol) using the MP2 energy as the true value (excluding α_L).

M05-2X/cc-pVTZ//M05-2X/6-31G**					M05-2X-D[a]/cc-pVTZ//M05-2X/6-31G**					M05-2X/6-31G**// M05-2X/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	1.40	-0.27	-0.34	-0.78	Pro	-2.74	1.51	2.99	-1.76	Pro	-0.05	-0.27	-0.25	0.57
Gly	1.58	-0.12	-1.09	-0.37	Gly	-0.91	0.52	-0.09	0.48	Gly	0.06	0.46	-0.83	0.31
Ala	1.43	-0.25	-0.48	-0.71	Ala	-1.02	0.55	0.43	0.04	Ala	-0.02	0.24	-0.08	-0.14
Val	1.37	-0.07	-0.65	-0.65	Val	-0.85	0.28	0.16	0.41	Val	-0.02	0.63	-0.36	-0.25
Leu	1.30	-0.12	-0.67	-0.50	Leu	-0.81	0.41	0.08	0.32	Leu	-0.27	0.58	-0.54	0.23
Ile	1.29	-0.12	-0.63	-0.54	Ile	-0.59	0.45	0.52	-0.39	Ile	-0.15	0.57	-0.20	-0.22
Met	1.17	-0.26	-0.52	-0.39	Met	-0.86	0.48	0.33	0.05	Met	-0.32	0.30	-0.16	0.17
Phe	1.66	-0.18	-0.69	-0.79	Phe	0.08	-0.32	-0.68	0.92	Phe	0.34	0.00	-0.48	0.14
Tyr	1.81	-0.51	-0.76	-0.54	Tyr	0.21	-0.77	-0.77	1.34	Tyr	0.64	-0.28	-0.81	0.45
His	1.51	-0.30	-0.51	-0.70	His	0.07	-0.76	-0.27	0.97	His	0.13	-0.18	-0.24	0.28
Trp	1.99	-0.67	-0.63	-0.69	Trp	-0.60	0.93	-1.01	0.67	Trp	0.32	-0.22	-0.29	0.20
Cys	0.74	1.32	-1.00	-1.06	Cys	-1.59	1.97	-0.12	-0.27	Cys	-0.69	1.91	-0.84	-0.38
Ser	1.27	-0.11	-0.75	-0.42	Ser	-0.98	0.79	0.24	-0.06	Ser	-0.15	0.48	-0.45	0.12
Thr	1.13	-0.17	-0.56	-0.39	Thr	-0.92	0.48	0.32	0.12	Thr	-0.45	0.77	-0.24	-0.08
Asn	1.23	-0.60	-0.09	-0.54	Asn	-0.58	0.15	0.12	0.32	Asn	-0.10	-0.39	0.30	0.19
Gln	1.27	-0.29	-0.78	-0.20	Gln	-1.02	0.80	0.35	-0.13	Gln	-0.24	0.26	-0.64	0.62
Asp	0.51	-0.17	-0.09	-0.26	Asp	-1.31	0.95	-0.36	0.73	Asp	0.04	-1.01	-0.23	1.20
Glu	0.94	0.71	-1.12	-0.53	Glu	-1.56	1.45	-0.22	0.33	Glu	0.22	-0.47	-0.30	0.55
Lys	1.39	-0.06	-0.58	-0.76	Lys	-0.22	-0.53	0.57	0.19	Lys	-0.25	0.68	-0.39	-0.03
Arg	1.32	-0.25	0.16	-1.24	Arg	-0.05	-0.83	0.66	0.22	Arg	0.30	0.41	-0.61	-0.09

[a] AMBER99 dispersion correction.

M05-2X-D[a]/6-31G**// M05-2X/6-31G**					PBE/cc-pVTZ//PBE/6-31G**					PBE-D[a]/cc-pVTZ//PBE/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-4.19	1.51	3.09	-0.41	Pro	4.15	-2.32	-1.55	-0.28	Pro	0.01	-0.54	1.78	-1.26
Gly	-2.44	1.11	0.17	1.16	Gly	4.41	-2.33	-2.52	0.45	Gly	1.91	-1.69	-1.52	1.30
Ala	-2.47	1.03	0.83	0.61	Ala	4.31	-2.57	-2.16	0.42	Ala	1.85	-1.77	-1.25	1.17
Val	-2.24	0.98	0.45	0.82	Val	4.15	-2.38	-1.81	0.04	Val	1.93	-2.03	-1.01	1.10
Leu	-2.38	1.12	0.20	1.05	Leu	4.25	-2.36	-2.01	0.11	Leu	2.14	-1.82	-1.26	0.93
Ile	-2.03	1.14	0.96	-0.07	Ile	3.97	-2.42	-1.83	0.28	Ile	2.09	-1.85	-0.67	0.43
Met	-2.35	1.05	0.69	0.61	Met	3.77	-2.54	-2.05	0.82	Met	1.74	-1.79	-1.21	1.26
Phe	-1.24	-0.14	-0.47	1.85	Phe	4.09	-1.78	-1.66	-0.66	Phe	2.52	-1.92	-1.65	1.05
Tyr	-0.96	-0.54	-0.82	2.33	Tyr	3.93	-1.59	-1.68	-0.66	Tyr	2.33	-1.85	-1.70	1.22
His	-1.31	-0.64	0.00	1.95	His	4.33	-1.82	-2.00	-0.50	His	2.88	-2.28	-1.76	1.16
Trp	-2.27	1.38	-0.67	1.56	Trp	4.73	-2.54	-1.82	-0.36	Trp	2.14	-0.94	-2.20	1.00
Cys	-3.02	2.56	0.05	0.41	Cys	3.94	-2.18	-1.89	0.13	Cys	1.62	-1.53	-1.01	0.92
Ser	-2.40	1.38	0.54	0.48	Ser	4.11	-2.40	-2.08	0.37	Ser	1.86	-1.50	-1.09	0.73
Thr	-2.50	1.42	0.65	0.44	Thr	4.30	-2.43	-2.05	0.18	Thr	2.25	-1.78	-1.16	0.70
Asn	-1.92	0.36	0.50	1.06	Asn	3.88	-2.05	-1.76	-0.07	Asn	2.07	-1.31	-1.56	0.80
Gln	-2.53	1.35	0.49	0.69	Gln	3.61	-2.65	-2.24	1.28	Gln	1.31	-1.56	-1.11	1.36
Asp	-1.78	0.10	-0.51	2.18	Asp	2.19	-0.94	0.00	-1.25	Asp	0.37	0.18	-0.28	-0.27
Glu	-2.29	0.28	0.61	1.40	Glu	3.83	-1.26	-2.28	-0.29	Glu	1.33	-0.52	-1.38	0.56
Lys	-1.86	0.20	0.75	0.91	Lys	4.36	-2.53	-1.96	0.13	Lys	2.74	-3.01	-0.81	1.08
Arg	-1.08	-0.17	-0.11	1.37	Arg	3.23	-2.51	-0.71	-0.01	Arg	1.86	-3.09	-0.21	1.44

[a] AMBER99 dispersion correction.

PBE/6-31G**// PBE/6-31G**					PBE-D[a]/6-31G**// PBE/6-31G**					B3LYP/cc-pVTZ//B3LYP/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	2.45	-2.21	-1.33	1.09	Pro	-1.69	-0.43	2.01	0.11	Pro	5.03	-2.16	-1.65	-1.22
Gly	2.67	-1.57	-2.12	1.02	Gly	0.17	-0.93	-1.11	1.87	Gly	5.29	-2.47	-2.39	-0.43
Ala	2.65	-1.82	-1.62	0.78	Ala	0.20	-1.02	-0.71	1.53	Ala	5.30	-2.61	-2.45	-0.24
Val	2.52	-1.43	-1.34	0.25	Val	0.30	-1.08	-0.54	1.32	Val	5.04	-2.51	-2.01	-0.52
Leu	2.40	-1.39	-1.69	0.68	Leu	0.30	-0.85	-0.95	1.50	Leu	5.24	-2.43	-2.19	-0.62
Ile	2.34	-1.48	-1.35	0.49	Ile	0.46	-0.91	-0.20	0.65	Ile	4.92	-2.53	-1.97	-0.42
Met	2.10	-1.68	-1.54	1.13	Met	0.07	-0.93	-0.70	1.56	Met	4.65	-2.69	-2.36	0.41
Phe	2.49	-1.32	-1.09	-0.09	Phe	0.91	-1.46	-1.08	1.62	Phe	4.98	-1.66	-1.82	-1.50
Tyr	2.42	-1.29	-1.08	-0.05	Tyr	0.82	-1.55	-1.09	1.83	Tyr	4.86	-1.59	-1.75	-1.52
His	2.61	-1.28	-1.43	0.11	His	1.16	-1.74	-1.19	1.78	His	5.21	-1.68	-2.16	-1.37
Trp	2.90	-1.91	-1.19	0.19	Trp	0.32	-0.30	-1.57	1.55	Trp	5.83	-2.65	-1.99	-1.19
Cys	2.30	-1.40	-1.56	0.66	Cys	-0.03	-0.75	-0.68	1.45	Cys	4.95	-2.19	-2.09	-0.67
Ser	2.44	-1.61	-1.57	0.74	Ser	0.19	-0.72	-0.58	1.10	Ser	5.18	-2.62	-2.45	-0.10
Thr	2.38	-1.31	-1.51	0.44	Thr	0.33	-0.66	-0.62	0.96	Thr	5.31	-2.63	-2.24	-0.44
Asn	2.34	-1.57	-1.21	0.45	Asn	0.52	-0.83	-1.01	1.31	Asn	4.84	-2.22	-1.79	-0.82
Gln	1.89	-1.89	-1.89	1.89	Gln	-0.40	-0.80	-0.76	1.97	Gln	4.51	-2.76	-2.53	0.79
Asp	1.30	-1.90	0.43	0.16	Asp	-0.52	-0.79	0.16	1.15	Asp	2.50	-0.78	-0.11	-1.61
Glu	2.89	-2.05	-1.33	0.49	Glu	0.39	-1.31	-0.42	1.34	Glu	4.24	-0.25	-2.81	-1.18
Lys	2.46	-1.66	-1.52	0.72	Lys	0.85	-2.13	-0.37	1.66	Lys	5.39	-2.57	-2.15	-0.66
Arg	2.15	-1.45	-1.73	1.03	Arg	0.78	-2.03	-1.23	2.49	Arg	3.97	-2.67	-0.18	-1.12

[a] AMBER99 dispersion correction.

B3LYP-D[a]/cc-pVTZ//B3LYP/6-31G**					B3LYP/6-31G**// B3LYP/6-31G**					B3LYP-D[a]/6-31G**// B3LYP/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	0.89	-0.38	1.69	-2.20	Pro	3.29	-2.03	-1.41	0.15	Pro	-0.85	-0.25	1.92	-0.83
Gly	2.79	-1.82	-1.39	0.42	Gly	3.44	-1.76	-1.89	0.20	Gly	0.95	-1.11	-0.88	1.05
Ala	2.85	-1.82	-1.54	0.51	Ala	3.58	-1.90	-1.92	0.24	Ala	1.13	-1.10	-1.02	0.99
Val	2.82	-2.16	-1.21	0.54	Val	3.34	-1.60	-1.55	-0.20	Val	1.12	-1.24	-0.74	0.87
Leu	3.14	-1.90	-1.44	0.20	Leu	3.32	-1.52	-1.87	0.07	Leu	1.21	-0.98	-1.13	0.89
Ile	3.04	-1.96	-0.82	-0.27	Ile	3.20	-1.64	-1.53	-0.04	Ile	1.32	-1.07	-0.37	0.12
Met	2.62	-1.94	-1.52	0.84	Met	2.93	-1.87	-1.88	0.82	Met	0.90	-1.13	-1.03	1.26
Phe	3.40	-1.80	-1.81	0.21	Phe	3.27	-1.19	-1.25	-0.83	Phe	1.69	-1.33	-1.24	0.88
Tyr	3.26	-1.85	-1.76	0.36	Tyr	3.12	-0.99	-1.25	-0.89	Tyr	1.52	-1.25	-1.26	0.99
His	3.77	-2.14	-1.92	0.29	His	3.37	-1.12	-1.62	-0.63	His	1.93	-1.58	-1.38	1.03
Trp	3.25	-1.05	-2.37	0.17	Trp	3.85	-1.93	-1.41	-0.52	Trp	1.27	-0.32	-1.79	0.84
Cys	2.62	-1.54	-1.21	0.13	Cys	3.25	-1.42	-1.78	-0.05	Cys	0.92	-0.77	-0.90	0.74
Ser	2.93	-1.73	-1.46	0.26	Ser	3.47	-1.87	-1.95	0.35	Ser	1.22	-0.97	-0.96	0.71
Thr	3.26	-1.98	-1.36	0.07	Thr	3.33	-1.53	-1.70	-0.10	Thr	1.28	-0.88	-0.81	0.42
Asn	3.02	-1.47	-1.59	0.04	Asn	3.23	-1.82	-1.26	-0.16	Asn	1.42	-1.07	-1.05	0.70
Gln	2.21	-1.67	-1.40	0.86	Gln	2.75	-2.03	-2.20	1.48	Gln	0.45	-0.94	-1.06	1.55
Asp	0.68	0.34	-0.39	-0.63	Asp	1.67	-1.73	0.11	-0.06	Asp	-0.15	-0.61	-0.16	0.92
Glu	1.73	0.50	-1.90	-0.33	Glu	3.05	-0.99	-1.88	-0.18	Glu	0.55	-0.25	-0.97	0.67
Lys	3.77	-3.05	-1.01	0.28	Lys	3.40	-1.72	-1.70	0.02	Lys	1.79	-2.20	-0.56	0.97
Arg	2.59	-3.25	0.32	0.33	Arg	2.81	-1.63	-1.16	-0.02	Arg	1.43	-2.21	-0.66	1.43

[a] AMBER99 dispersion correction.

AM1// AM1					AM1-D[a]// AM1					PM3// PM3				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	3.30	-2.90	-0.40	-0.01	Pro	-0.84	-1.11	2.94	-0.99	Pro	8.40	-2.97	-2.83	-2.60
Gly	3.90	-2.58	-0.50	-0.81	Gly	1.40	-1.94	0.50	0.04	Gly	7.34	-1.11	-0.74	-5.49
Ala	3.36	-2.41	0.11	-1.07	Ala	0.91	-1.61	1.02	-0.32	Ala	7.84	-2.36	-0.32	-5.16
Val	2.86	-1.98	0.60	-1.48	Val	0.64	-1.63	1.40	-0.41	Val	7.80	-2.40	-0.18	-5.23
Leu	3.83	-2.06	-0.20	-1.57	Leu	1.72	-1.52	0.55	-0.75	Leu	8.90	-2.47	-0.55	-5.88
Ile	2.86	-1.73	0.74	-1.87	Ile	0.98	-1.16	1.90	-1.72	Ile	7.67	-2.14	-0.19	-5.34
Met	1.86	-2.33	0.22	0.24	Met	-0.17	-1.58	1.06	0.68	Met	6.48	-2.41	-0.48	-3.58
Phe	4.08	-1.89	0.46	-2.65	Phe	2.50	-2.03	0.47	-0.95	Phe	7.91	-1.05	-0.08	-6.78
Tyr	3.94	-1.78	0.53	-2.69	Tyr	2.34	-2.04	0.51	-0.81	Tyr	7.94	-1.45	0.14	-6.63
His	4.05	-1.93	0.20	-2.31	His	2.60	-2.40	0.44	-0.64	His	8.22	-1.83	-0.33	-6.06
Trp	4.53	-2.16	0.11	-2.47	Trp	1.94	-0.56	-0.27	-1.11	Trp	8.61	-1.79	-0.39	-6.43
Cys	2.69	-1.20	-0.13	-1.36	Cys	0.36	-0.55	0.75	-0.57	Cys	6.91	-1.57	-0.06	-5.28
Ser	2.08	-2.34	2.25	-1.99	Ser	-0.16	-1.44	3.24	-1.63	Ser	5.83	0.00	-0.96	-4.86
Thr	2.37	-2.16	0.17	-0.38	Thr	0.32	-1.51	1.05	0.13	Thr	9.13	-2.91	-1.55	-4.67
Asn	2.21	-0.39	-0.26	-1.55	Asn	0.39	0.36	-0.06	-0.69	Asn	6.19	-0.16	-0.46	-5.57
Gln	1.60	-2.63	-0.24	1.26	Gln	-0.69	-1.54	0.90	1.33	Gln	6.01	-2.81	-0.75	-2.45
Asp	1.62	1.14	-0.24	-2.52	Asp	-0.20	2.25	-0.51	-1.54	Asp	6.92	2.16	-3.65	-5.43
Glu	3.68	1.13	-1.98	-2.83	Glu	1.18	1.87	-1.08	-1.98	Glu	7.65	1.16	-2.58	-6.23
Lys	3.40	-2.25	0.13	-1.28	Lys	1.79	-2.72	1.27	-0.33	Lys	7.83	-2.53	-0.23	-5.06
Arg	-0.11	-3.88	6.35	-2.36	Arg	-1.49	-4.46	6.85	-0.91	Arg	4.23	-4.13	5.11	-5.20

[a] AMBER99 dispersion correction.

PM3-D[a]//PM3					PM3MM// PM3MM					PM3MM-D[a]// PM3MM				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	4.26	-1.19	0.51	-3.58	Pro	8.48	-3.42	-3.03	-2.03	Pro	4.34	-1.64	0.31	-3.01
Gly	4.85	-0.47	0.26	-4.64	Gly	8.33	-3.07	-1.21	-4.06	Gly	5.84	-2.42	-0.20	-3.21
Ala	5.39	-1.57	0.59	-4.41	Ala	8.11	-3.03	-0.85	-4.22	Ala	5.66	-2.24	0.05	-3.47
Val	5.58	-2.04	0.63	-4.17	Val	7.88	-2.94	-0.51	-4.42	Val	5.66	-2.59	0.29	-3.36
Leu	6.79	-1.93	0.20	-5.06	Leu	9.00	-3.12	-0.89	-4.99	Leu	6.90	-2.59	-0.14	-4.17
Ile	5.79	-1.57	0.96	-5.18	Ile	7.79	-2.77	-0.56	-4.46	Ile	5.91	-2.20	0.60	-4.31
Met	4.45	-1.67	0.36	-3.14	Met	6.71	-3.11	-0.97	-2.63	Met	4.68	-2.37	-0.12	-2.19
Phe	6.33	-1.19	-0.07	-5.07	Phe	8.34	-2.31	-0.20	-5.83	Phe	6.76	-2.45	-0.19	-4.12
Tyr	6.34	-1.71	0.12	-4.76	Tyr	8.17	-2.17	-0.11	-5.88	Tyr	6.57	-2.43	-0.13	-4.01
His	6.78	-2.29	-0.09	-4.40	His	8.29	-2.30	-0.51	-5.48	His	6.85	-2.76	-0.27	-3.81
Trp	6.02	-0.19	-0.76	-5.07	Trp	8.77	-2.56	-0.46	-5.75	Trp	6.18	-0.96	-0.84	-4.39
Cys	4.58	-0.92	0.82	-4.48	Cys	7.67	-2.00	-1.49	-4.19	Cys	5.35	-1.35	-0.61	-3.39
Ser	3.58	0.89	0.03	-4.50	Ser	7.04	-3.28	1.17	-4.93	Ser	4.79	-2.38	2.16	-4.57
Thr	7.07	-2.26	-0.66	-4.15	Thr	9.99	-3.33	-3.78	-2.89	Thr	7.94	-2.68	-2.89	-2.38
Asn	4.37	0.59	-0.26	-4.70	Asn	7.15	-1.60	-0.87	-4.68	Asn	5.34	-0.85	-0.67	-3.82
Gln	3.71	-1.72	0.39	-2.38	Gln	6.53	-3.39	-1.48	-1.66	Gln	4.24	-2.30	-0.35	-1.58
Asp	5.10	3.28	-3.93	-4.45	Asp	6.31	2.70	-2.88	-6.13	Asp	4.49	3.82	-3.16	-5.15
Glu	5.15	1.91	-1.68	-5.38	Glu	7.03	0.95	-2.55	-5.43	Glu	4.52	1.70	-1.64	-4.57
Lys	6.21	-3.01	0.92	-4.12	Lys	8.89	-3.51	-1.03	-4.35	Lys	7.28	-3.98	0.11	-3.40
Arg	2.85	-4.71	5.61	-3.74	Arg	5.67	-5.15	4.19	-4.71	Arg	4.29	-5.73	4.69	-3.25

[a] AMBER99 dispersion correction.

AMOEBA// AMOEBA					AMBEREP// AMBEREP					AMBERPOL// AMBERPOL				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-3.58	2.02	5.44	-3.88	Pro	-4.08	2.77	2.73	-1.43	Pro	-4.77	3.66	4.07	-2.95
Gly	0.22	0.50	0.48	-1.19	Gly	0.17	-0.46	-1.73	2.03	Gly	-0.21	0.66	0.39	-0.84
Ala	0.32	0.35	0.53	-1.20	Ala	-1.07	0.54	-0.24	0.77	Ala	-1.42	1.46	1.11	-1.14
Val	-0.21	1.02	1.73	-2.54	Val	-0.48	0.39	-0.35	0.45	Val	-0.77	1.07	0.88	-1.18
Leu	-0.04	0.06	1.16	-1.18	Leu	-1.08	1.01	-0.76	0.83	Leu	-1.40	1.81	0.42	-0.83
Ile	-0.70	0.59	1.42	-1.31	Ile	-0.74	0.76	-0.17	0.15	Ile	-1.17	1.61	1.16	-1.60
Met	-0.45	0.62	0.44	-0.61	Met	-1.87	0.58	-0.38	1.67	Met	-2.21	1.37	0.93	-0.08
Phe	-0.45	0.30	0.60	-0.44	Phe	-1.11	0.58	-0.17	0.71	Phe	-1.35	1.24	0.97	-0.85
Tyr	-0.24	0.11	0.40	-0.27	Tyr	-0.84	0.26	-0.57	1.15	Tyr	-1.20	1.06	0.92	-0.78
His	2.61	-0.46	-0.64	-1.51	His	0.68	-0.69	-0.20	0.20	His	-0.05	0.35	0.80	-1.09
Trp	0.21	0.95	0.53	-1.69	Trp	-2.23	1.65	-0.05	0.63	Trp	-2.51	2.49	1.06	-1.03
Cys	1.00	-0.06	0.48	-1.41	Cys	-2.17	3.12	0.00	-0.95	Cys	-1.58	2.92	0.40	-1.74
Ser	-0.76	0.67	0.05	0.03	Ser	-1.20	0.81	-0.64	1.03	Ser	-1.20	1.42	0.40	-0.62
Thr	2.26	0.11	0.69	-3.06	Thr	-0.79	1.34	0.73	-1.28	Thr	-1.70	1.60	1.51	-1.40
Asn	2.08	0.24	-2.37	0.05	Asn	-0.75	1.78	-2.36	1.33	Asn	-0.18	1.89	-1.49	-0.22
Gln	0.34	-0.26	-0.15	0.06	Gln	-1.00	0.91	0.01	0.08	Gln	-1.17	1.58	1.18	-1.60
Asp	-1.19	4.24	-0.83	-2.22	Asp	-1.47	1.98	-1.81	1.31	Asp	-1.08	2.46	-0.96	-0.41
Glu	-1.17	2.84	1.02	-2.69	Glu	-4.13	3.69	-1.14	1.58	Glu	-4.07	4.28	0.14	-0.35
Lys	1.74	-0.58	0.75	-1.91	Lys	-0.18	0.07	-0.36	0.48	Lys	-0.62	0.31	1.10	-0.78
Arg	-0.59	0.82	0.95	-1.18	Arg	-1.69	-0.89	2.87	-0.29	Arg	-2.38	-0.14	3.92	-1.40

AMBER94// AMBER94					AMBER96// AMBER96					AMBER99// AMBER99				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-5.40	1.87	5.39	-1.86	Pro	0.68	-0.61	1.49	-1.57	Pro	-3.81	2.26	2.10	-0.55
Gly	-2.01	1.09	1.42	-0.50	Gly	4.08	-1.38	-2.48	-0.21	Gly	-0.78	1.89	-1.75	0.65
Ala	-3.08	1.87	2.19	-0.98	Ala	3.00	-0.61	-1.71	-0.69	Ala	-1.52	2.27	-1.06	0.31
Val	-2.50	1.48	1.80	-0.78	Val	3.58	-1.00	-2.09	-0.49	Val	-0.93	1.86	-1.45	0.51
Leu	-3.24	0.93	2.54	-0.23	Leu	2.84	-1.54	-1.36	0.06	Leu	-1.70	1.30	-0.66	1.06
Ile	-2.04	1.85	2.31	-2.12	Ile	4.04	-0.62	-1.58	-1.83	Ile	-0.44	2.23	-0.96	-0.83
Met	-3.59	1.77	1.70	0.13	Met	2.49	-0.71	-2.19	0.42	Met	-2.02	2.15	-1.56	1.42
Phe	-3.09	1.62	2.07	-0.60	Phe	2.99	-0.85	-1.82	-0.32	Phe	-1.52	2.02	-1.18	0.68
Tyr	-2.79	1.37	1.99	-0.57	Tyr	3.29	-1.10	-1.91	-0.28	Tyr	-1.22	1.76	-1.26	0.72
His	-3.15	1.38	2.60	-0.83	His	2.93	-1.10	-1.30	-0.54	His	-1.58	1.77	-0.65	0.46
Trp	-3.51	2.55	1.86	-0.91	Trp	2.57	0.07	-2.03	-0.62	Trp	-1.93	2.94	-1.39	0.39
Cys	-3.69	3.77	1.79	-1.88	Cys	2.39	1.30	-2.10	-1.59	Cys	-2.12	4.17	-1.45	-0.59
Ser	-3.02	2.51	2.22	-1.71	Ser	3.06	0.04	-1.68	-1.42	Ser	-1.47	2.91	-1.03	-0.41
Thr	-3.18	1.04	1.62	0.52	Thr	2.91	-1.44	-2.27	0.81	Thr	-1.60	1.43	-1.64	1.81
Asn	-1.82	0.27	1.94	-0.40	Asn	4.27	-2.21	-1.95	-0.11	Asn	-0.43	0.45	-0.74	0.72
Gln	-3.44	2.26	2.29	-1.11	Gln	2.64	-0.21	-1.61	-0.82	Gln	-2.04	2.50	-1.13	0.67
Asp	-4.64	3.20	0.86	0.58	Asp	1.44	0.72	-3.04	0.87	Asp	-3.12	3.75	-2.44	1.81
Glu	-6.00	5.22	0.47	0.31	Glu	0.08	2.75	-3.43	0.60	Glu	-4.43	5.61	-2.79	1.61
Lys	-2.66	1.71	2.72	-1.77	Lys	3.42	-0.77	-1.17	-1.49	Lys	-1.07	2.10	-0.54	-0.49
Arg	-4.18	0.80	6.13	-2.76	Arg	1.91	-1.68	2.24	-2.47	Arg	-2.64	1.13	3.03	-1.53

AMBER99SB// AMBER99SB					AMBER03// AMBER03					CHARMM27// CHARMM27				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	1.59	1.55	0.79	-3.92	Pro	-0.03	3.22	0.44	-3.62	Pro	0.33	1.28	2.34	-3.94
Gly	3.48	0.52	-1.23	-2.77	Gly	2.11	0.40	-0.54	-1.97	Gly	3.15	-1.73	-0.80	-0.61
Ala	3.55	0.49	-1.25	-2.79	Ala	1.91	0.91	-0.54	-2.28	Ala	1.37	-0.32	1.02	-2.07
Val	4.15	0.11	-1.63	-2.63	Val	3.07	-0.05	-1.58	-1.45	Val	1.46	-0.63	1.32	-2.15
Leu	3.36	-0.48	-0.85	-2.04	Leu	1.79	0.30	0.02	-2.11	Leu	1.81	-0.89	1.44	-2.36
Ile	4.67	0.51	-1.10	-4.07	Ile	4.41	0.08	-1.26	-3.23	Ile	1.66	-0.40	1.62	-2.89
Met	3.03	0.37	-1.74	-1.66	Met	0.82	1.31	-0.48	-1.65	Met	1.10	-0.42	0.59	-1.26
Phe	3.52	0.24	-1.36	-2.40	Phe	1.12	1.00	-0.18	-1.94	Phe	2.64	-0.74	0.82	-2.72
Tyr	3.82	-0.01	-1.42	-2.39	Tyr	-1.21	1.75	0.75	-1.30	Tyr	2.75	-0.88	0.76	-2.63
His	3.51	0.01	-0.80	-2.72	His	-1.83	2.01	1.50	-1.68	His	3.03	-0.81	0.99	-3.21
Trp	3.12	1.14	-1.54	-2.73	Trp	-1.06	1.63	0.47	-1.03	Trp	1.92	-0.52	0.78	-2.18
Cys	2.95	2.25	-1.61	-3.59	Cys	1.03	2.90	-0.67	-3.26	Cys	1.34	1.13	0.65	-3.13
Ser	3.62	1.12	-1.24	-3.50	Ser	1.85	1.41	-0.83	-2.42	Ser	1.02	-0.70	0.01	-0.33
Thr	4.06	-0.35	-1.84	-1.88	Thr	3.84	0.14	-0.13	-3.84	Thr	1.58	-1.24	0.89	-1.23
Asn	4.47	-1.36	-0.70	-2.41	Asn	1.66	-0.54	0.41	-1.53	Asn	1.76	1.23	-0.42	-2.57
Gln	2.86	0.58	-1.48	-1.96	Gln	3.71	0.27	-1.84	-2.13	Gln	1.00	-0.30	0.79	-1.48
Asp	1.87	2.02	-2.59	-1.31	Asp	-0.93	3.10	-2.38	0.21	Asp	-4.36	6.63	0.57	-2.84
Glu	0.64	3.87	-2.96	-1.54	Glu	1.68	3.98	-3.83	-1.83	Glu	-2.72	3.98	0.74	-2.00
Lys	3.99	0.34	-0.72	-3.61	Lys	5.51	-0.27	-0.25	-4.99	Lys	2.60	-1.04	1.15	-2.70
Arg	2.41	-0.64	2.90	-4.67	Arg	0.35	-0.85	6.05	-5.55	Arg	1.21	-2.02	5.09	-4.28

OPLS-AA// OPLS-AA					OPLS-AA/L// OPLS-AA/L					AMBERUA// AMBERUA				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-0.57	-1.28	6.60	-4.75	Pro	-0.69	-0.29	7.21	-6.23	Pro	0.41	1.55	2.31	-4.27
Gly	3.40	-1.46	-1.38	-0.57	Gly	6.51	-3.36	-3.29	0.14	Gly	2.32	0.30	-0.83	-1.79
Ala	3.43	-1.61	-0.78	-1.04	Ala	3.22	-0.24	-0.89	-2.09	Ala	0.26	1.55	0.06	-1.88
Val	3.62	-1.52	-0.54	-1.57	Val	3.28	-0.23	-0.76	-2.29	Val	1.69	1.42	0.09	-3.20
Leu	3.93	-2.05	-0.64	-1.24	Leu	3.84	-0.48	-0.79	-2.57	Leu	-0.07	1.29	0.31	-1.53
Ile	4.14	-1.05	0.04	-3.12	Ile	3.04	-0.51	-0.90	-1.63	Ile	0.52	1.67	0.33	-2.52
Met	2.63	-2.50	-2.03	1.90	Met	2.45	-1.22	-2.13	0.90	Met	-0.11	1.38	-0.05	-1.21
Phe	4.61	-2.04	-0.71	-1.85	Phe	4.36	-0.72	-0.63	-3.01	Phe	0.38	1.52	0.12	-2.02
Tyr	4.68	-2.15	-0.76	-1.78	Tyr	4.42	-0.87	-0.63	-2.93	Tyr	-2.60	2.38	1.15	-0.93
His	4.10	-1.88	-0.54	-1.68	His	3.92	-0.73	-0.49	-2.70	His	-0.37	1.67	0.73	-2.03
Trp	2.74	-2.69	0.36	-0.41	Trp	2.81	-1.10	0.06	-1.77	Trp	-1.07	2.35	0.50	-1.78
Cys	3.80	-0.88	-1.59	-1.33	Cys	4.25	-0.13	-2.41	-1.71	Cys	-0.48	3.33	-0.13	-2.71
Ser	3.78	-1.84	-1.53	-0.41	Ser	4.54	0.55	-0.97	-4.12	Ser	-1.09	1.52	-0.43	-0.01
Thr	4.18	-1.39	-0.15	-2.65	Thr	3.71	-0.20	-0.22	-3.30	Thr	1.23	0.09	-1.11	-0.21
Asn	5.11	-5.04	-0.06	0.00	Asn	4.63	-0.67	-2.33	-1.63	Asn	1.85	-0.39	0.29	-1.75
Gln	2.98	-0.21	0.21	-2.98	Gln	3.33	-0.11	-0.63	-2.58	Gln	1.19	1.82	-0.06	-2.94
Asp	0.41	-2.79	2.43	-0.05	Asp	-1.96	2.38	1.47	-1.89	Asp	-1.06	2.47	-0.58	-0.83
Glu	0.65	3.26	-2.07	-1.84	Glu	-1.47	2.85	-0.30	-1.08	Glu	-0.31	4.37	-2.24	-1.82
Lys	5.51	-2.57	-1.09	-1.86	Lys	4.66	-1.07	-0.92	-2.66	Lys	0.20	1.36	0.68	-2.24
Arg	2.59	-3.21	4.05	-3.43	Arg	2.65	-1.88	3.77	-4.54	Arg	-0.24	-0.56	5.27	-4.47

GROMOS(G43b1)// GROMOS(G43b1)					GROMOS(G45a3)// GROMOS(G45a3)					GROMOS(G53a6)// GROMOS(G53a6)				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	2.35	-1.23	2.10	-3.22	Pro	3.08	-1.60	1.64	-3.11	Pro	0.30	-4.18	11.41	-7.53
Gly	5.41	-3.57	-1.28	-0.56	Gly	5.65	-3.76	-1.46	-0.43	Gly	7.67	-4.58	-2.75	-0.34
Ala	5.13	-3.58	-0.85	-0.70	Ala	5.42	-3.86	-1.11	-0.46	Ala	7.45	-4.66	-2.37	-0.43
Val	5.11	-3.26	-0.19	-1.65	Val	5.26	-3.52	-0.28	-1.46	Val	7.18	-4.48	-1.45	-1.25
Leu	5.45	-3.62	-1.10	-0.74	Leu	5.59	-4.21	-0.95	-0.43	Leu	7.97	-4.86	-1.84	-1.27
Ile	4.96	-3.28	-0.16	-1.52	Ile	4.91	-3.67	-0.27	-0.97	Ile	6.93	-4.51	-1.31	-1.11
Met	4.54	-3.58	-0.85	-0.10	Met	4.68	-3.88	-1.04	0.23	Met	5.70	-4.31	-1.98	0.58
Phe	5.07	-3.45	-1.27	-0.36	Phe	5.46	-3.77	-1.47	-0.21	Phe	7.56	-4.62	-2.40	-0.54
Tyr	5.13	-3.45	-1.79	0.11	Tyr	5.38	-3.84	-1.77	0.23	Tyr	7.49	-4.69	-2.72	-0.08
His	4.93	-2.84	-0.73	-1.36	His	5.06	-3.28	-0.38	-1.40	His	6.79	-4.94	-1.12	-0.72
Trp	3.52	-1.71	-0.94	-0.87	Trp	3.84	-1.88	-1.10	-0.85	Trp	6.03	-2.82	-1.80	-1.41
Cys	5.17	-2.02	-1.19	-1.97	Cys	5.42	-2.29	-1.35	-1.78	Cys	7.13	-2.98	-2.86	-1.29
Ser	4.19	-3.11	-0.87	-0.20	Ser	4.42	-3.39	-1.06	0.03	Ser	6.53	-3.54	-1.86	-1.13
Thr	5.20	-3.29	-0.96	-0.95	Thr	5.32	-3.70	-1.12	-0.49	Thr	7.17	-3.77	-1.18	-2.22
Asn	5.55	-2.19	-2.32	-1.04	Asn	5.79	-2.39	-2.53	-0.86	Asn	7.14	-3.97	-1.88	-1.29
Gln	4.41	-2.84	-0.21	-1.37	Gln	4.50	-3.30	-0.49	-0.72	Gln	6.50	-3.58	-1.30	-1.62
Asp	10.40	3.11	-3.44	-10.07	Asp	4.44	5.80	-3.71	-6.54	Asp	4.78	3.84	-3.87	-4.74
Glu	3.89	6.99	-4.08	-6.80	Glu	2.11	8.28	-4.42	-5.97	Glu	4.17	5.20	-5.03	-4.34
Lys	5.49	-4.98	-1.06	0.54	Lys	5.09	-5.10	-0.53	0.54	Lys	6.98	-5.36	-1.53	-0.10
Arg	-3.01	-6.27	10.28	-0.99	Arg	0.58	-6.81	7.97	-1.74	Arg	3.63	-7.20	5.90	-2.32

Table S4c. Signed RMS-C excluding α_L (RMS-C-Nα_L, kcal/mol) of each conformation over 20 amino acids for each method.

	α_R	β	β_a	PPII	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.36	-0.44	-0.67	-0.65	0.78	0.34
M05-2X-D[a]/cc-pVTZ	-1.05	0.87	0.81	0.66	0.85	0.14
M05-2X/6-31G**	-0.30	0.64	-0.47	0.41	0.45	0.12
M05-2X-D[a]/6-31G**	-2.27	1.10	0.88	1.24	1.38	0.53
PBE/cc-pVTZ	4.01	-2.23	-1.88	0.55	2.17	1.24
PBE-D[a]/cc-pVTZ	1.97	-1.79	-1.32	1.03	1.53	0.37
PBE/6-31G**	2.41	-1.63	-1.47	0.77	1.57	0.58
PBE-D[a]/6-31G**	0.66	-1.17	-0.96	1.52	1.07	0.31
B3LYP/cc-pVTZ	4.91	-2.28	-2.07	-0.95	2.55	1.45
B3LYP-D[a]/cc-pVTZ	2.85	-1.86	-1.49	0.64	1.71	0.79
B3LYP/6-31G**	3.21	-1.64	-1.62	0.52	1.75	0.96
B3LYP-D[a]/6-31G**	1.23	-1.18	-1.07	0.94	1.11	0.11
AM1	3.11	-2.17	1.61	-1.83	2.18	0.57
AM1-D[a]	1.38	-1.92	2.01	-1.02	1.58	0.40
PM3	7.48	-2.19	-1.73	-5.32	4.18	2.35
PM3-D[a]	5.38	-2.03	1.65	-4.43	3.37	1.57
PM3MM	7.87	-2.96	-1.85	-4.61	4.32	2.27
PM3MM-D[a]	5.78	-2.69	-1.58	-3.71	3.44	1.55
AMOEBA	1.38	1.32	1.54	-1.76	1.50	0.17
AMBEREP	-1.75	1.56	-1.25	1.06	1.40	0.26
AMBERPOL	-1.94	1.97	1.55	-1.22	1.67	0.31
AMBER94	-3.51	2.22	2.63	-1.25	2.40	0.81
AMBER96	2.92	-1.23	-2.05	-1.07	1.82	0.74
AMBER99	-2.08	2.58	-1.59	0.99	1.81	0.59
AMBER99SB	3.37	1.29	-1.62	-2.87	2.29	0.86
AMBER03	2.43	1.75	-1.87	-2.73	2.19	0.40
CHARMM27	2.15	1.98	1.53	-2.53	2.05	0.36
OPLS-AA	3.62	-2.31	2.06	-2.09	2.52	0.64
OPLS-AA/L	3.71	-1.34	-2.25	-2.82	2.53	0.86
AMBERUA	1.14	1.92	1.47	-2.30	1.71	0.44
GROMOS(G43b1)	5.17	-3.67	-2.82	-2.97	3.66	0.93
GROMOS(G45a3)	4.78	-4.21	-2.48	-2.26	3.43	1.08
GROMOS(G53a6)	6.50	-4.50	-3.66	-2.48	4.29	1.47

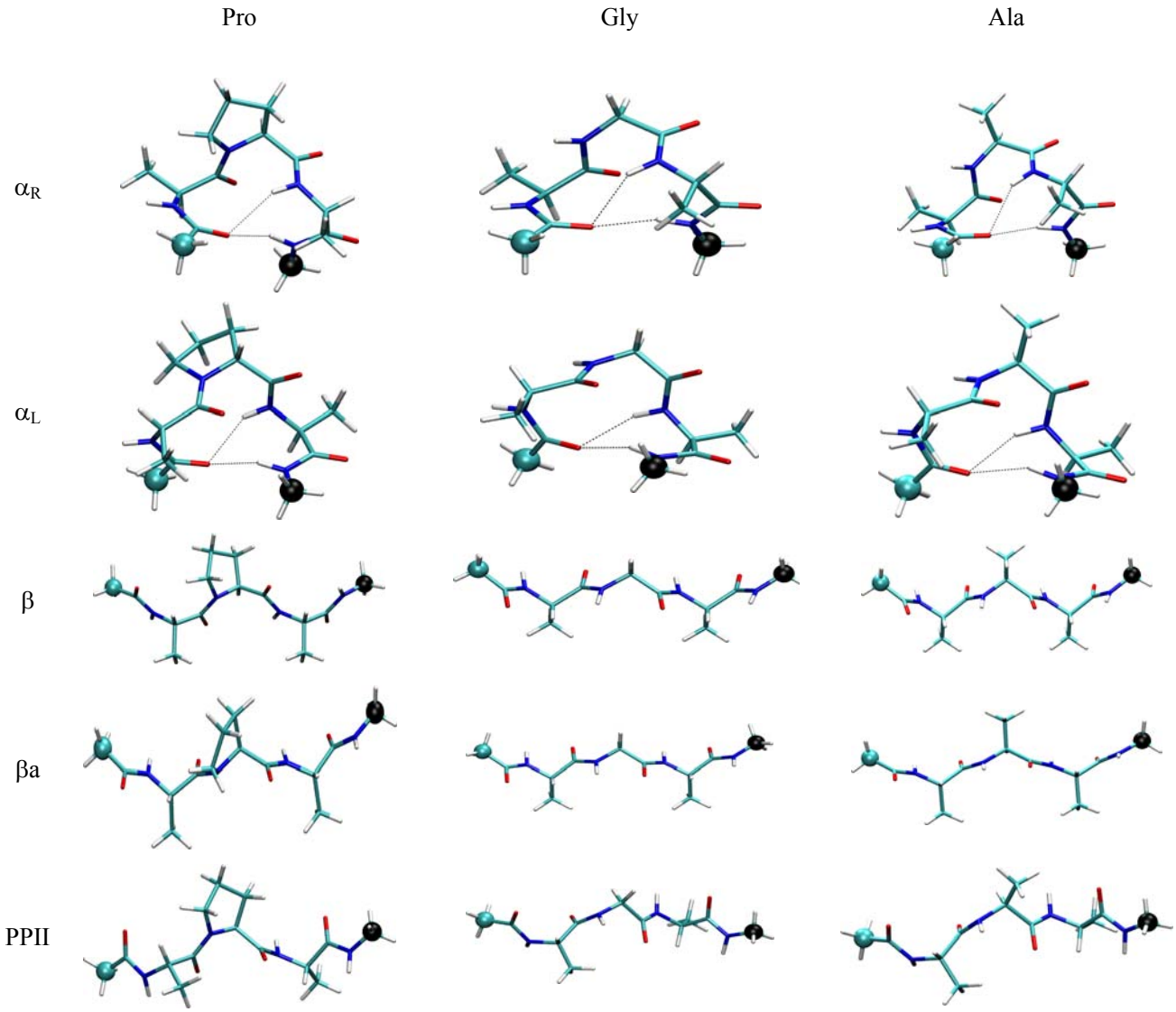
[1] Standard deviation. [a] AMBER99 dispersion correction.

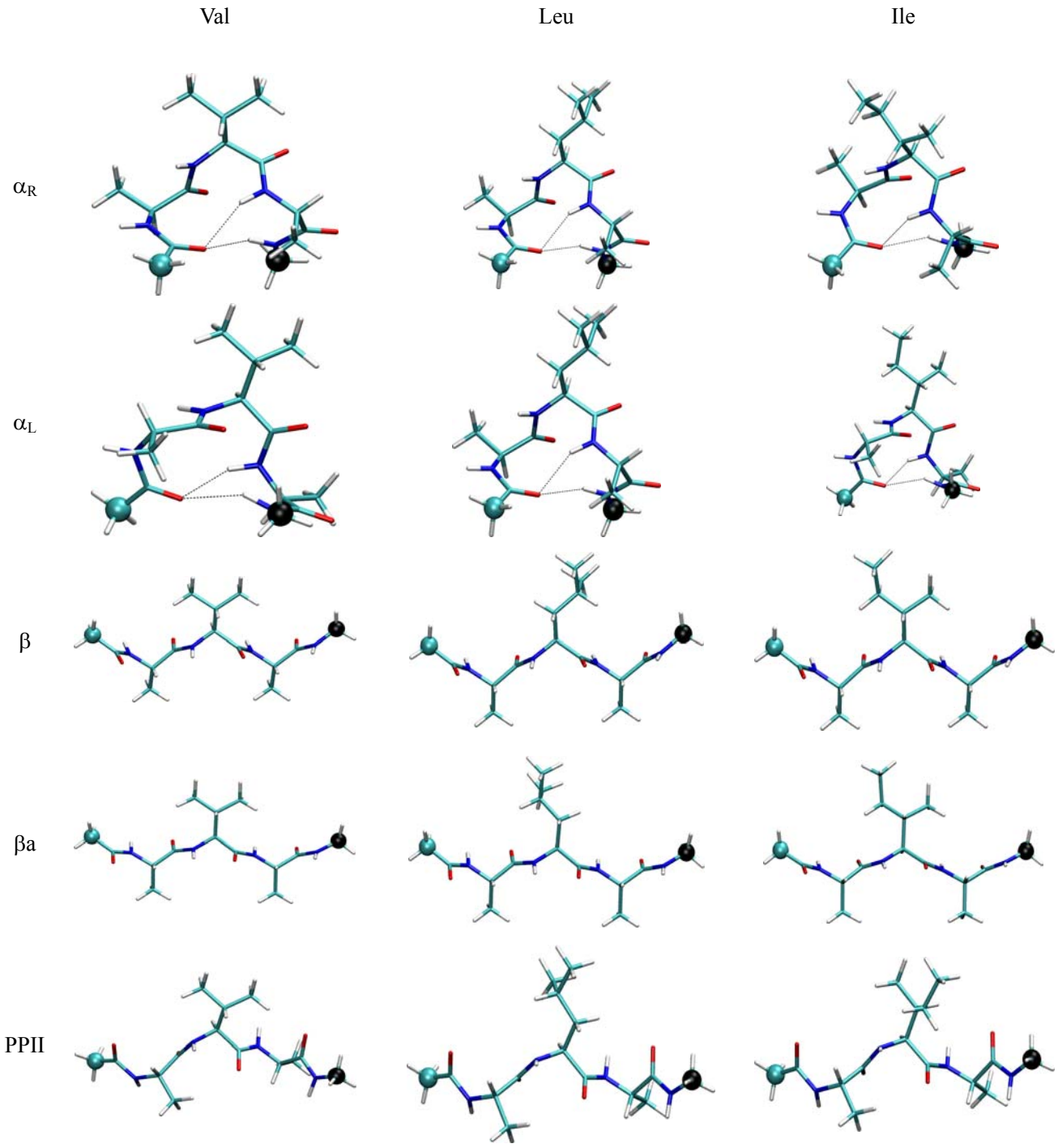
Table S4d. RMS over the four conformations (RMS-Nα_L, kcal/mol) for each tetrapeptide.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	0.83	0.98	0.84	0.83	0.77	0.77	0.68	0.99	1.05	0.88	1.15	1.05	0.77	0.67	0.74	0.77	0.30	0.85	0.84	0.92	0.83	0.17
M05-2X-D[a]/cc-pVTZ	2.34	0.58	0.62	0.50	0.48	0.49	0.52	0.59	0.87	0.63	0.82	1.27	0.64	0.55	0.35	0.68	0.91	1.08	0.42	0.54	0.74	0.43
M05-2X/6-31G**	0.34	0.50	0.14	0.38	0.44	0.33	0.25	0.30	0.58	0.22	0.26	1.11	0.34	0.46	0.27	0.48	0.79	0.40	0.41	0.40	0.42	0.21
M05-2X-D[a]/6-31G**	2.72	1.46	1.43	1.31	1.42	1.26	1.37	1.14	1.35	1.21	1.58	1.99	1.43	1.49	1.14	1.50	1.43	1.38	1.11	0.88	1.43	0.37
PBE/cc-pVTZ	2.51	2.80	2.74	2.56	2.63	2.50	2.53	2.40	2.31	2.56	2.84	2.44	2.60	2.68	2.37	2.59	1.35	2.32	2.70	2.08	2.48	0.31
PBE-D[a]/cc-pVTZ	1.12	1.62	1.54	1.59	1.61	1.45	1.52	1.86	1.82	2.12	1.68	1.31	1.36	1.59	1.50	1.34	0.28	1.03	2.15	1.94	1.52	0.40
PBE/6-31G**	1.86	1.94	1.84	1.60	1.66	1.56	1.65	1.51	1.47	1.62	1.84	1.59	1.70	1.57	1.55	1.89	1.18	1.91	1.70	1.64	1.66	0.18
PBE-D[a]/6-31G**	1.33	1.18	0.99	0.90	0.99	0.61	0.98	1.30	1.38	1.50	1.12	0.88	0.72	0.68	0.96	1.15	0.75	0.98	1.43	1.76	1.08	0.29
B3LYP/cc-pVTZ	2.92	3.16	3.20	3.00	3.11	2.94	2.94	2.88	2.81	3.02	3.41	2.92	3.15	3.18	2.84	2.96	1.54	2.61	3.19	2.46	2.91	0.38
B3LYP-D[a]/cc-pVTZ	1.47	1.82	1.87	1.90	1.97	1.86	1.85	2.13	2.08	2.37	2.08	1.64	1.85	2.02	1.86	1.61	0.53	1.32	2.48	2.09	1.84	0.40
B3LYP/6-31G**	2.06	2.15	2.25	2.01	2.05	1.95	2.02	1.89	1.81	1.98	2.28	1.98	2.21	2.02	1.96	2.16	1.20	1.86	2.09	1.72	1.98	0.23
B3LYP-D[a]/6-31G**	1.14	1.00	1.06	1.01	1.06	0.87	1.09	1.32	1.27	1.52	1.18	0.84	0.98	0.90	1.09	1.08	0.56	0.66	1.52	1.53	1.08	0.25
AM1	2.20	2.39	2.14	1.91	2.31	1.95	1.50	2.62	2.56	2.52	2.80	1.62	2.17	1.62	1.37	1.67	1.61	2.59	2.14	3.90	2.18	0.57
AM1-D[a]	1.70	1.22	1.07	1.14	1.24	1.49	1.02	1.70	1.63	1.81	1.16	0.57	1.95	0.94	0.44	1.16	1.39	1.58	1.76	4.18	1.46	0.74
PM3	4.85	4.63	4.84	4.85	5.48	4.79	3.90	5.24	5.22	5.19	5.45	4.42	3.82	5.38	4.17	3.56	4.88	5.13	4.83	4.69	4.77	0.54
PM3-D[a]	2.85	3.37	3.58	3.64	4.35	3.99	2.85	4.10	4.06	4.20	3.96	3.26	2.91	4.27	3.23	2.37	4.24	3.93	4.04	4.35	3.68	0.58
PM3MM	4.92	4.92	4.84	4.76	5.40	4.70	3.96	5.22	5.15	5.11	5.40	4.55	4.64	5.78	4.37	3.85	4.82	4.64	5.28	4.96	4.86	0.46
PM3MM-D[a]	2.77	3.55	3.50	3.54	4.23	3.83	2.84	4.14	4.04	4.16	3.84	3.25	3.68	4.59	3.33	2.54	4.22	3.43	4.48	4.58	3.73	0.58
AMOEBA	3.92	0.70	0.70	1.62	0.83	1.07	0.53	0.46	0.27	1.56	1.01	0.90	0.51	1.94	1.58	0.23	2.50	2.10	1.38	0.91	1.24	0.87
AMBEREP	2.91	1.35	0.72	0.42	0.93	0.54	1.30	0.73	0.78	0.50	1.42	1.96	0.95	1.07	1.66	0.68	1.66	2.94	0.31	1.73	1.23	0.73
AMBERPOL	3.92	0.58	1.29	0.99	1.23	1.40	1.38	1.12	1.00	0.70	1.91	1.89	1.00	1.56	1.21	1.40	1.44	2.96	0.76	2.40	1.51	0.78
AMBER94	4.03	1.37	2.16	1.75	2.11	2.09	2.18	2.05	1.87	2.19	2.40	2.94	2.41	1.87	1.35	2.42	2.87	3.99	2.27	3.98	2.42	0.77
AMBER96	1.18	2.49	1.79	2.15	1.75	2.37	1.71	1.81	1.98	1.72	1.67	1.89	1.88	2.02	2.59	1.60	1.77	2.22	1.99	2.09	1.93	0.32
AMBER99	2.47	1.38	1.47	1.29	1.24	1.30	1.81	1.44	1.30	1.25	1.90	2.47	1.72	1.62	0.60	1.74	2.87	3.92	1.23	2.22	1.76	0.72
AMBER99SB	2.29	2.32	2.35	2.59	2.02	3.16	1.94	2.24	2.36	2.25	2.28	2.70	2.65	2.42	2.65	1.91	2.00	2.57	2.72	3.02	2.42	0.33
AMBER03	2.43	1.48	1.57	1.87	1.39	2.81	1.16	1.23	1.30	1.76	1.12	2.27	1.73	2.72	1.18	2.34	2.01	3.03	3.72	4.13	2.06	0.84
CHARMM27	2.38	1.86	1.35	1.49	1.71	1.86	0.91	1.97	1.99	2.30	1.53	1.82	0.64	1.26	1.69	0.99	4.22	2.64	2.03	3.53	1.91	0.82
OPLS-AA	4.13	2.00	2.00	2.13	2.33	2.65	2.29	2.71	2.75	2.42	1.94	2.21	2.24	2.57	3.59	2.11	1.86	2.16	3.23	3.36	2.53	0.59
OPLS-AA/L	4.78	4.02	1.97	2.04	2.36	1.80	1.79	2.69	2.71	2.42	1.75	2.59	3.11	2.49	2.74	2.13	1.95	1.70	2.77	3.37	2.56	0.77
AMBERUA	2.56	1.53	1.22	1.94	1.01	1.54	0.92	1.28	1.91	1.37	1.59	2.16	0.96	0.83	1.30	1.83	1.44	2.62	1.36	3.47	1.64	0.64
GROMOS(G43b1)	2.33	3.31	3.18	3.14	3.34	3.07	2.92	3.14	3.22	2.95	2.06	3.00	2.65	3.15	3.24	2.71	7.60	5.63	3.75	6.22	3.53	1.33
GROMOS(G45a3)	2.47	3.48	3.38	3.25	3.54	3.11	3.09	3.40	3.43	3.10	2.25	3.15	2.83	3.30	3.40	2.83	5.24	5.66	3.62	5.32	3.49	0.88
GROMOS(G53a6)	7.15	4.68	4.56	4.34	4.80	4.22	3.72	4.60	4.62	4.25	3.52	4.17	3.87	4.24	4.24	3.85	4.33	4.71	4.47	5.13	4.47	0.72

[1] Standard deviation. [a] AMBER99 dispersion correction.

Figure S1. Five conformations of each tetrapeptide. The H-bonds are indicated by dash lines. The N-and C-terminal are indicated by VDW balls in cyan and black, respectively.

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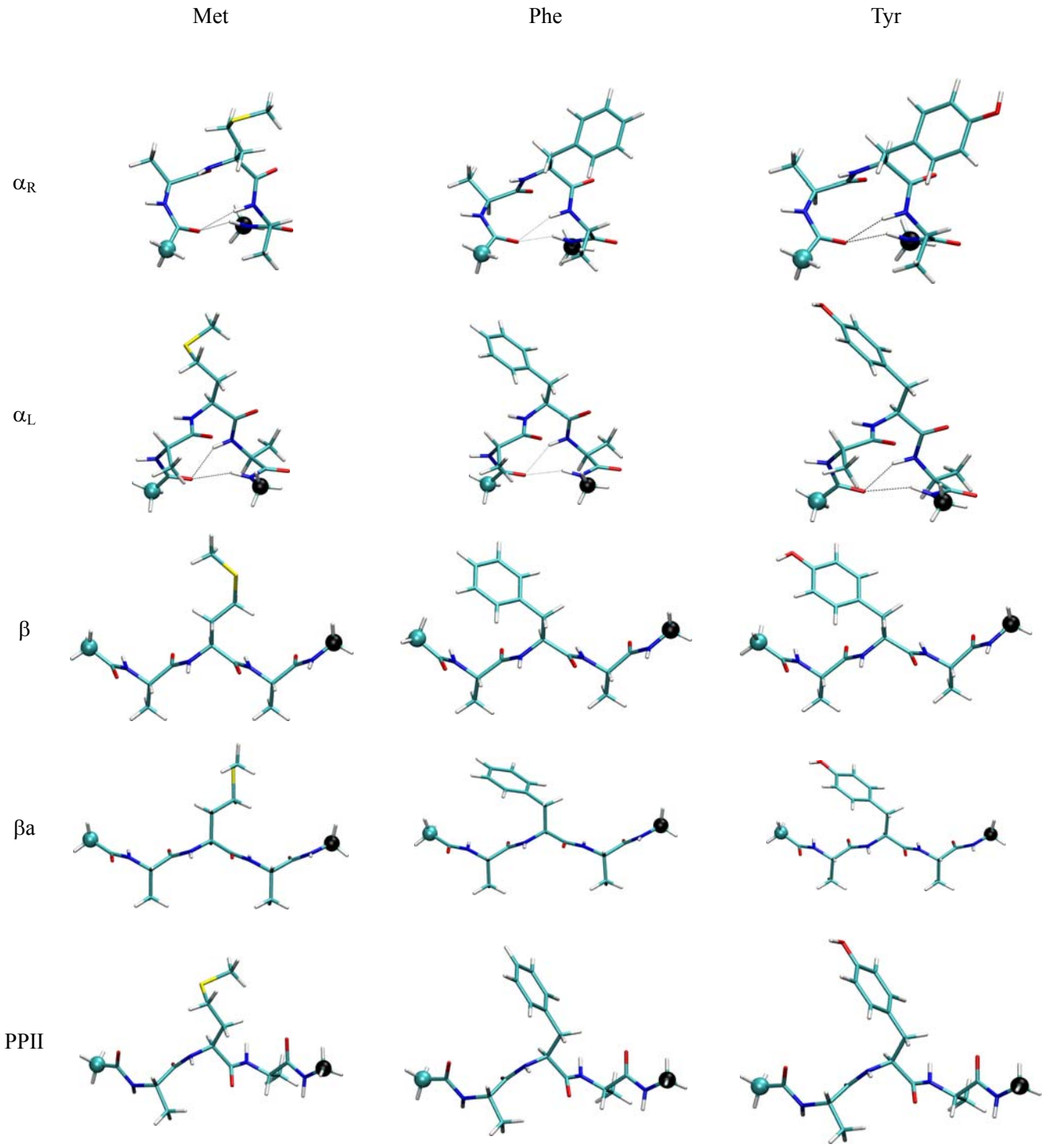
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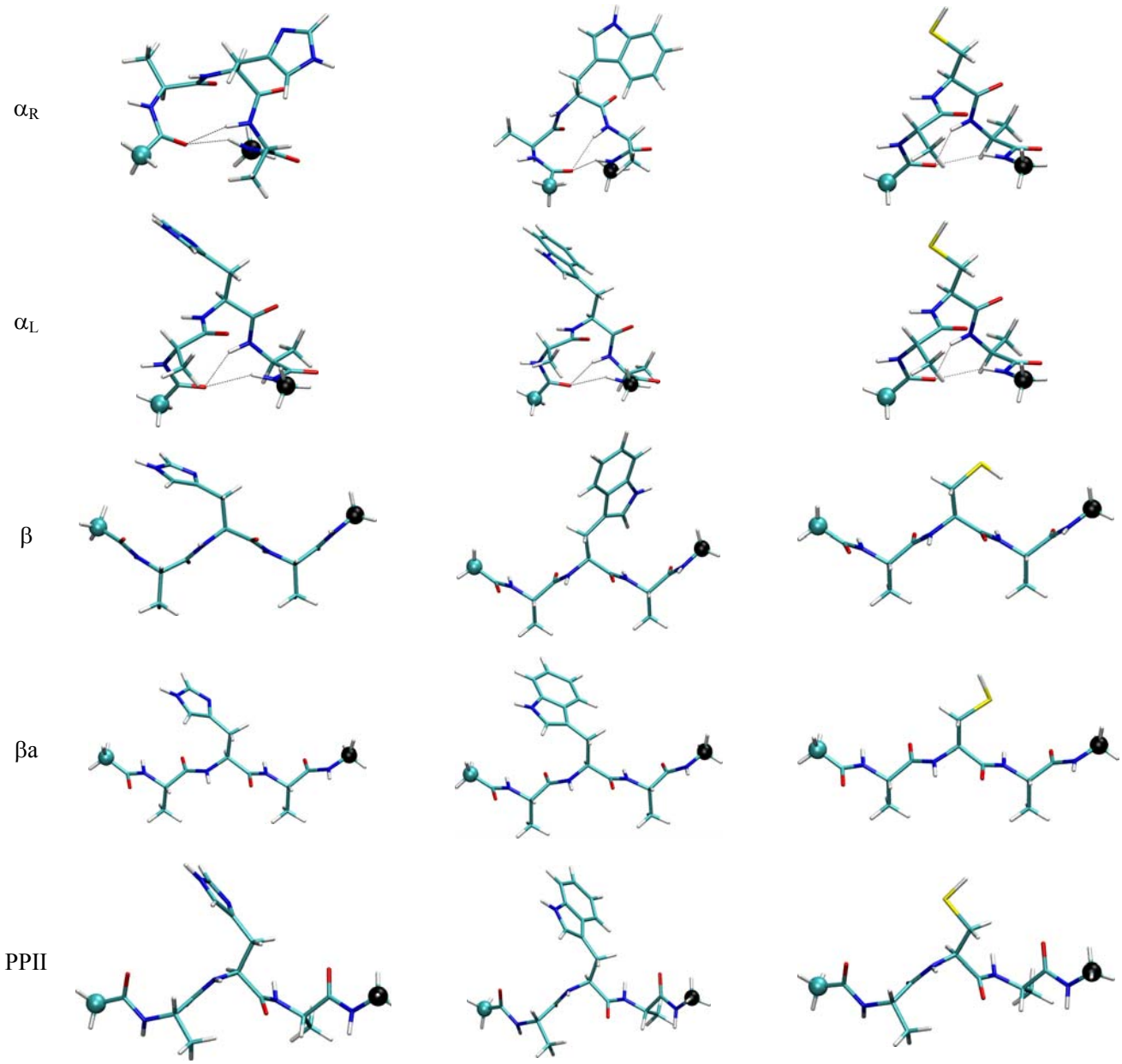
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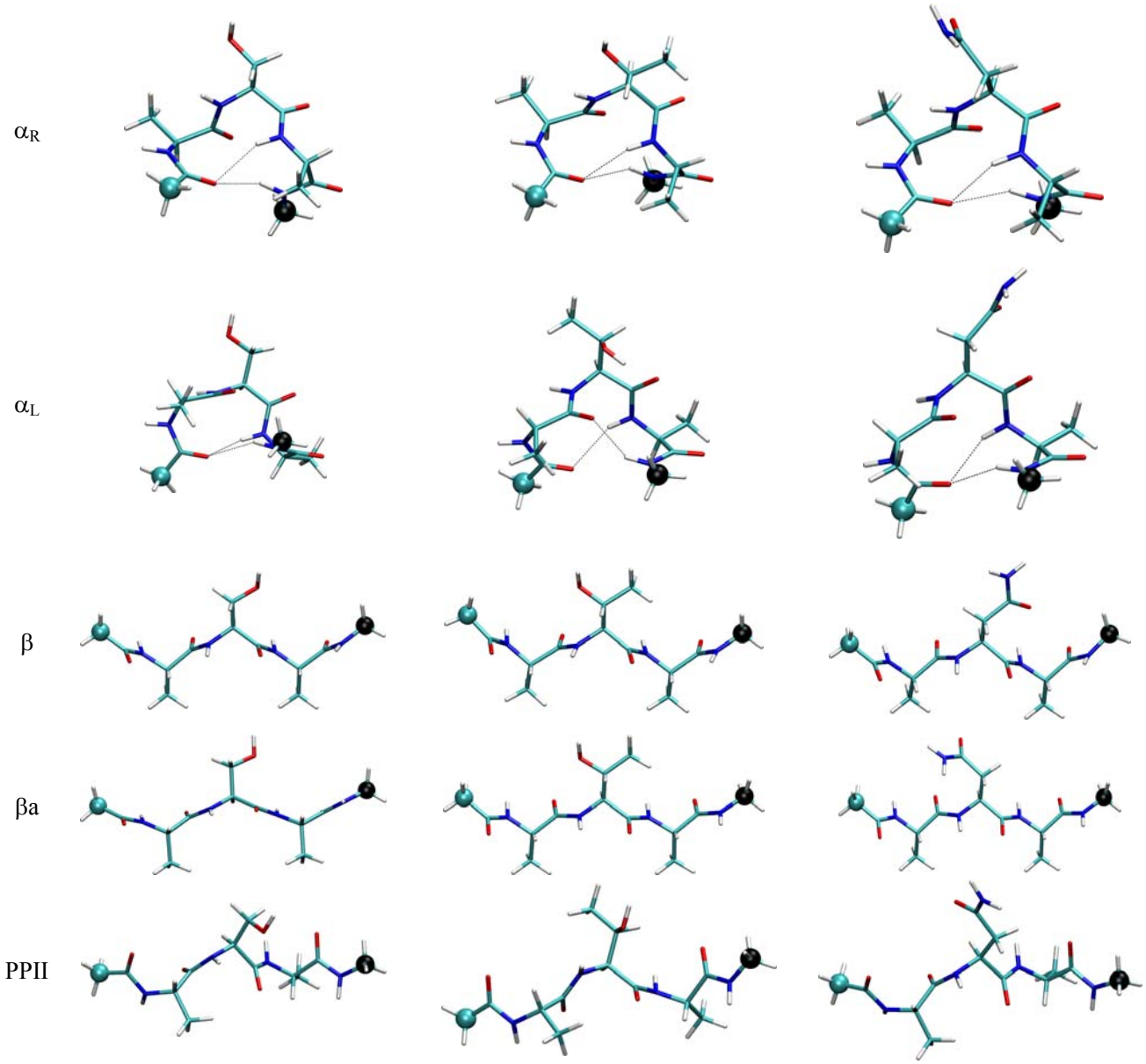
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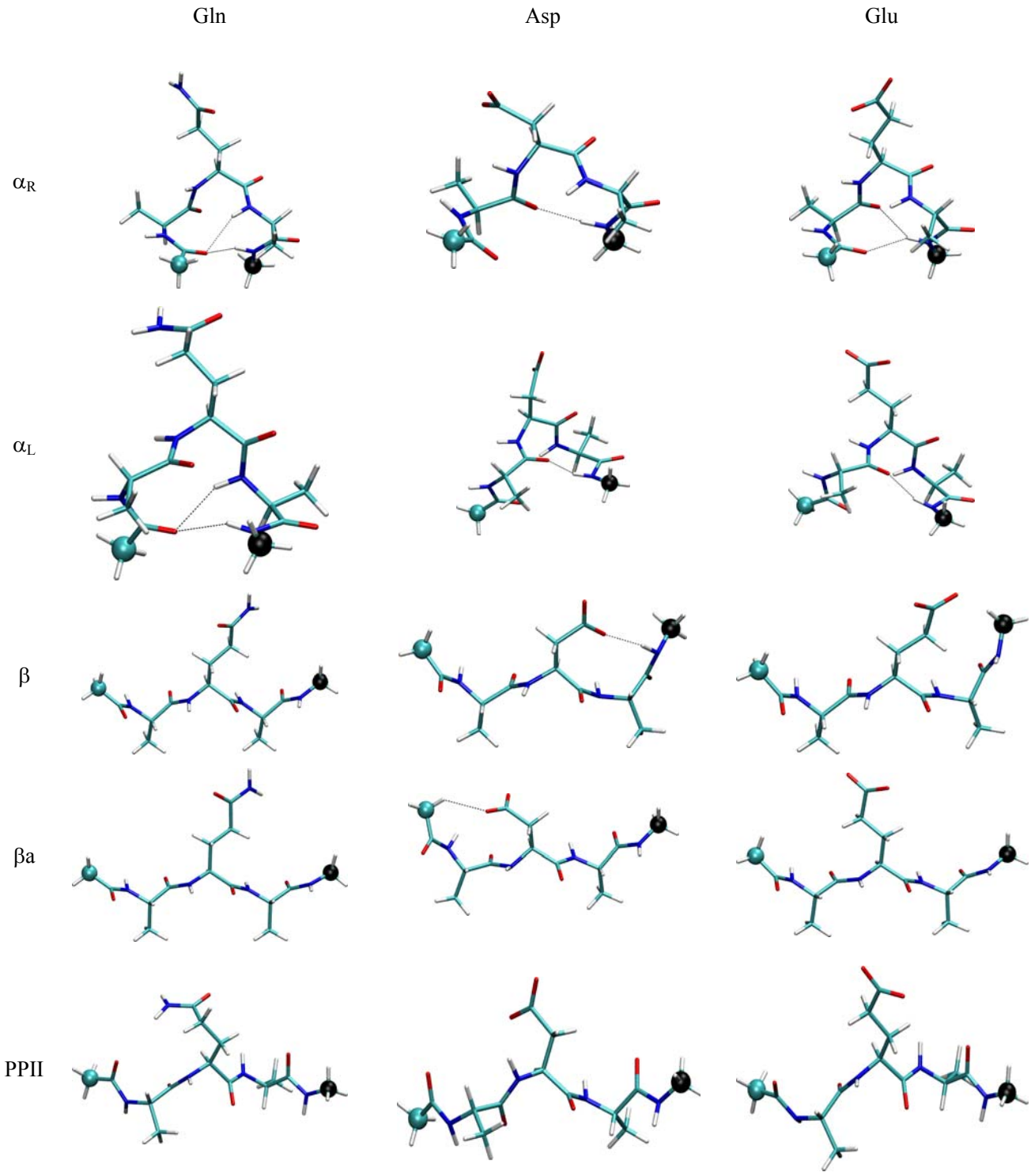
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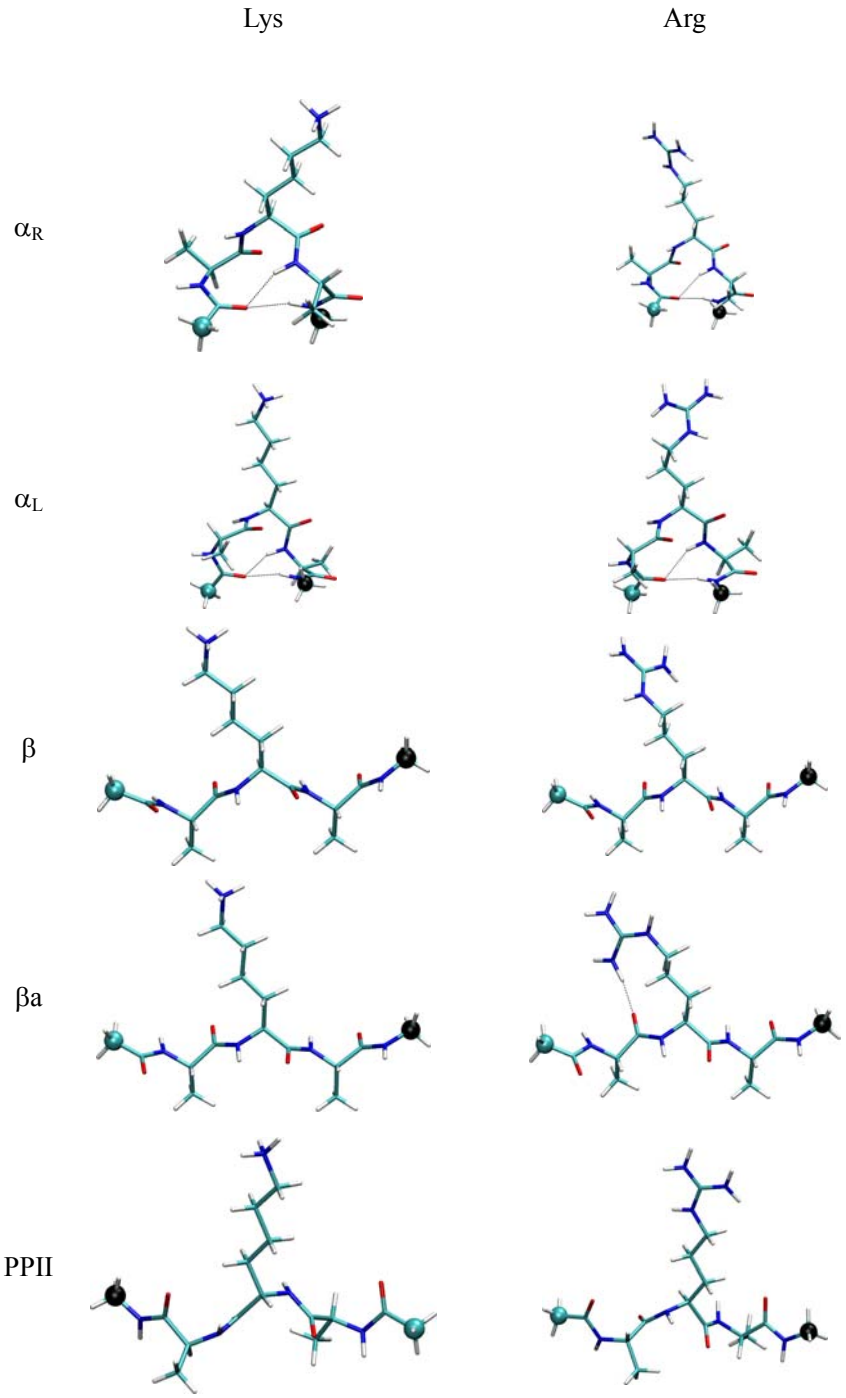
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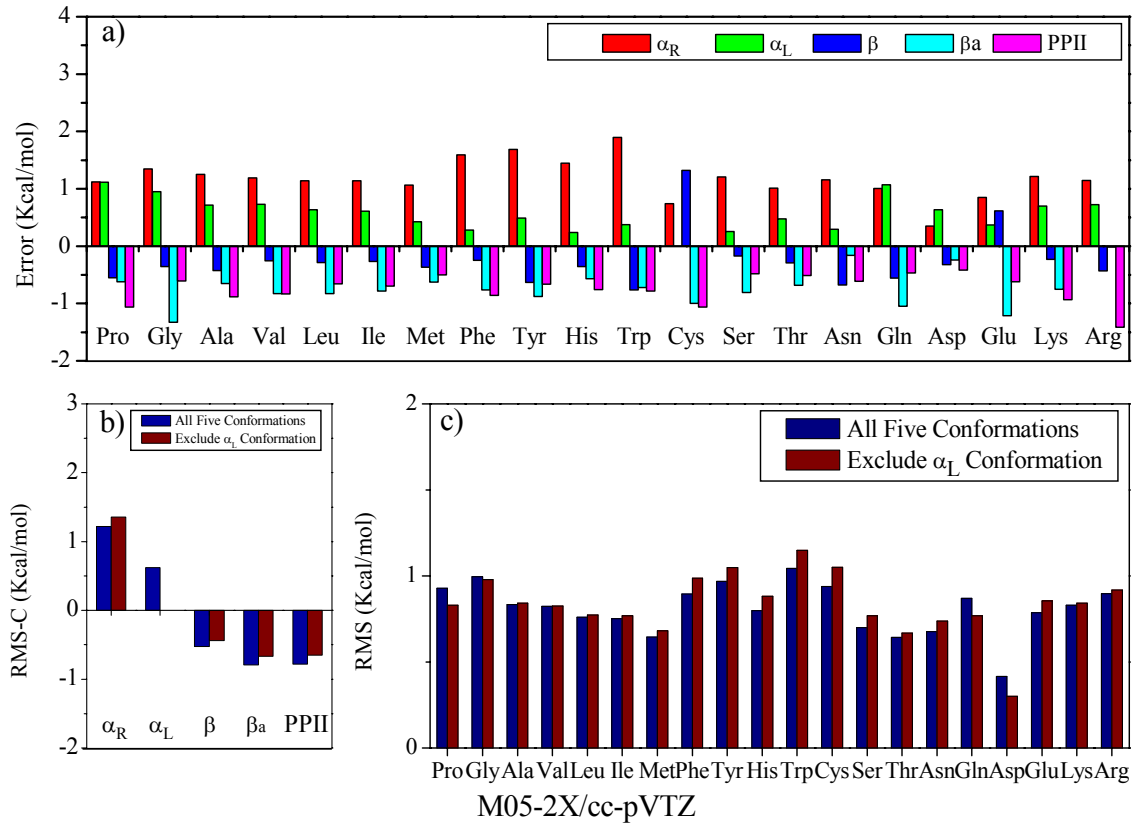

Figure S2. The performance of M05-2X/cc-PVTZ. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S2a - S2c show the performance of M05-2X/cc-PVTZ. First, this method overestimates the energies of the compact conformations (α_R and α_L) and underestimates those of the extended conformations (i.e. β (except for Cys and Glu), βa and PPII) (Fig. S2a). Thus, this method appears to overestimate the short range interactions (e.g. H-bond) and to underestimate the long range interactions (e.g. Dispersion energy). Second, the RMS-Cs using all five conformation data are 1.22, 0.62, -0.52, -0.79 and -0.78 kcal/mol for α_R, α_L, β, βa and PPII, respectively (Fig. S2b and Table S3c). Therefore, this method gives a good energetic description(<1.0 kcal/mol) over the latter four conformations but a slightly worse description for the former α_R. Third, this method gives a good energy description over twenty amino acids (Figure S2c and Table S3d) down to only 0.42 kcal/mol for ASP.

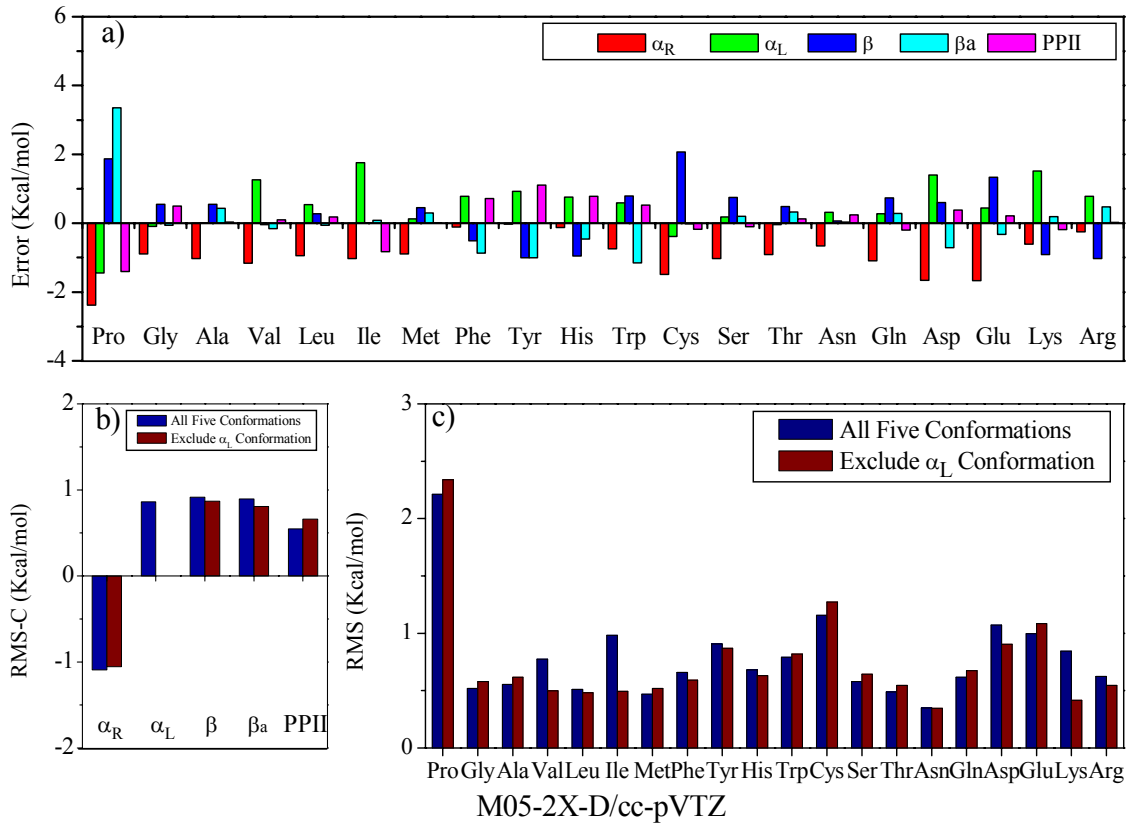

Figure S3.The performance of M05-2X/cc-PVTZ with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S3a – S3c show the performance of M05-2X/cc-PVTZ with the AMBER99 dispersion correction, RMS values become slightly smaller than the original ones (except for Pro).

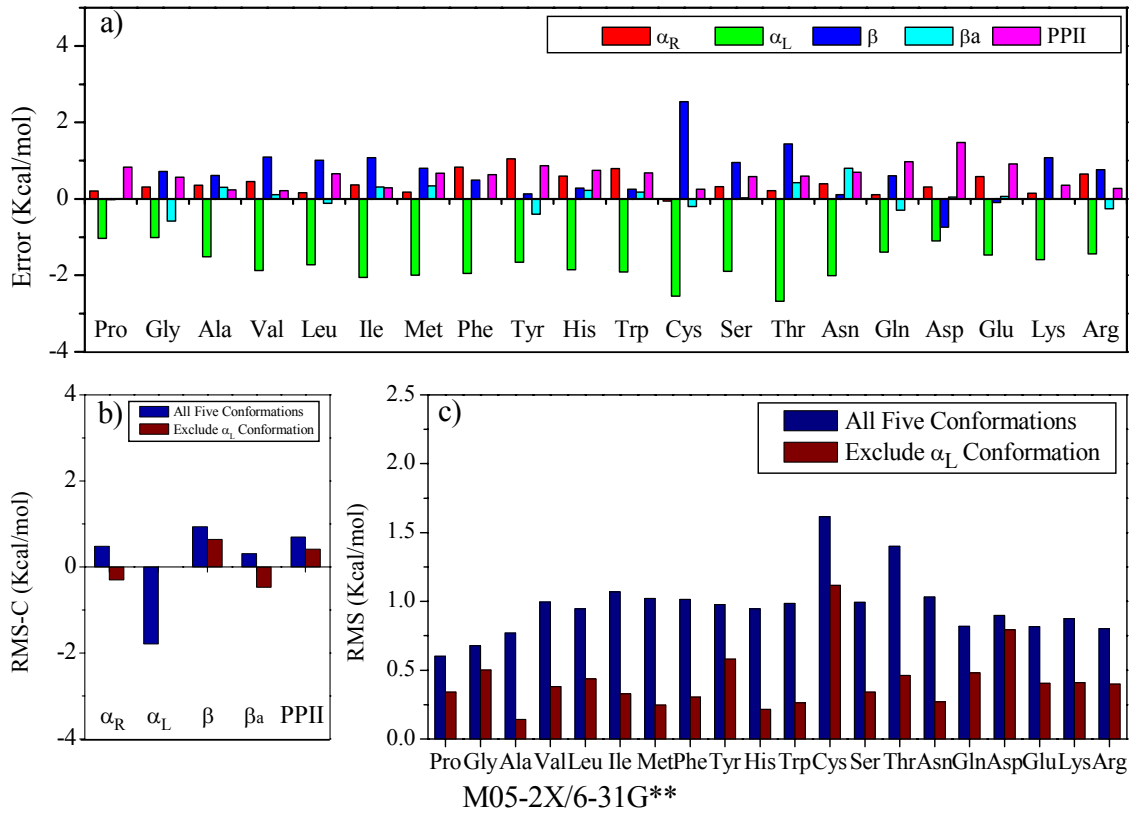

Figure S4. The performance of M05-2X/6-31G**. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S4a – S4c show the performance of M05-2X/6-31G**. This method significantly underestimates the energy of conformation α_L up to -2.68 kcal/mol of Thr; it slightly overestimates the energies of conformations βa (except for Gly, Leu, Tyr, Cys, Gln and Arg), β (except for Asp and glu), α_R and PPII. As a result, the RMS-C of α_L (-1.79 kcal/mol) is much higher than those of the other four conformations (0.48, 0.93, 0.31 and 0.70 kcal/mol for α_R, β, βa and PPII, respectively) (Table S3c and Fig. S4b). When α_L is excluded, this method gives a good energy description over all amino acids except for Cys and Asp (Figure S4c and Table S4d).

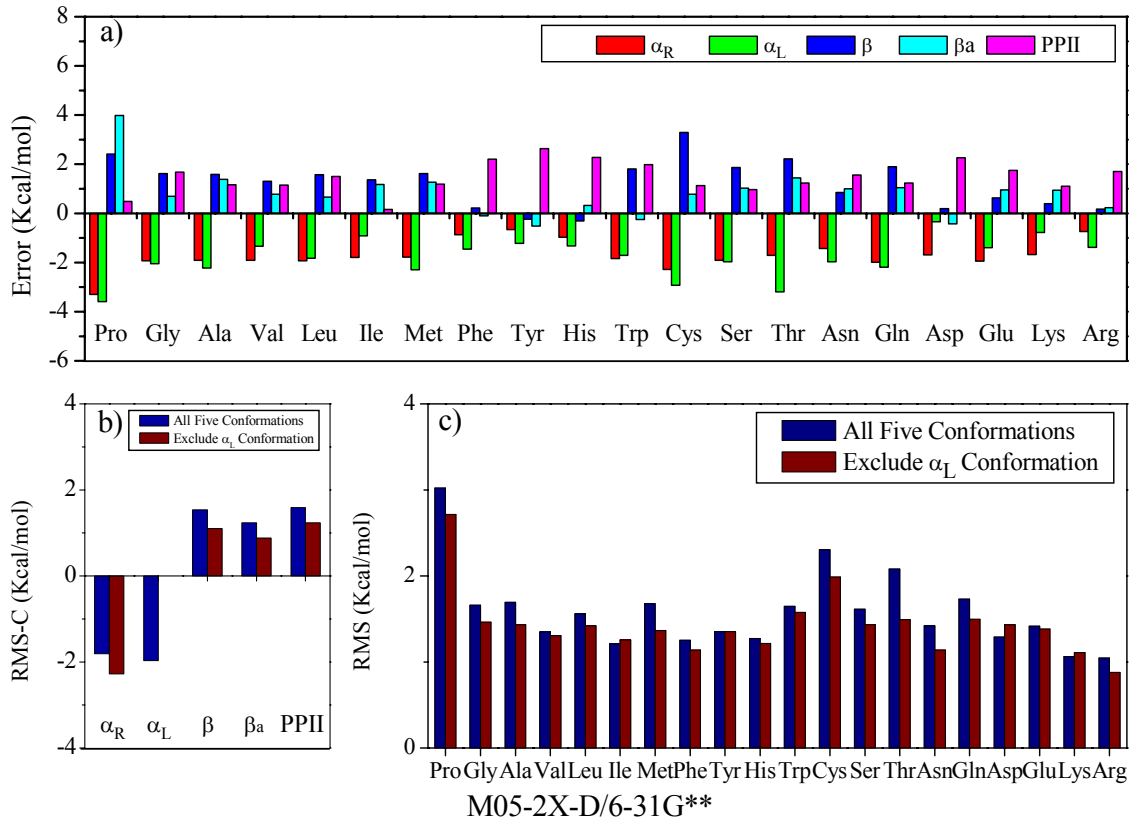

Figure S5. The performance of M05-2X/6-31G** with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S5a – S5c show the performance of M05-2X/6-31G** with the AMBER99 dispersion correction, the RMS values become even worse than the original values.

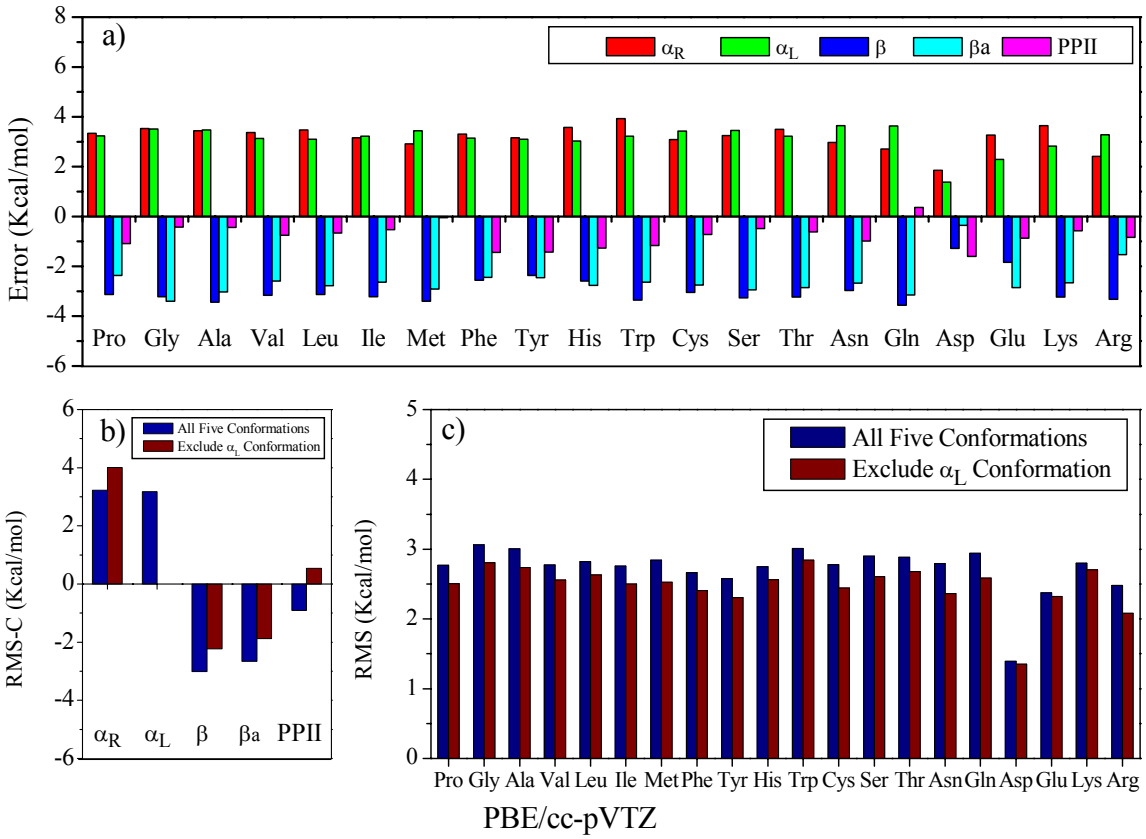

Figure S6. The performance of PBE/cc-pVTZ. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S6a – S6c show the performance of PBE/cc-pVTZ. First, this method overestimates the compact conformation energies (α_R and α_L) and underestimates the extended conformation energies (β, βa and PPII, except for the PPII conformations of Gln) in Fig. S6a. Thus, it appears to overestimate the short range interactions (e.g H-bond) and to underestimate the long range interactions (e.g Dispersion energy) (Fig. S6b). Second, the RMSs of the twenty amino acids all are ～ 3.0 kcal/mol and the RMS value of Asp is obviously smaller than others (Fig. S6c and Table S3d).

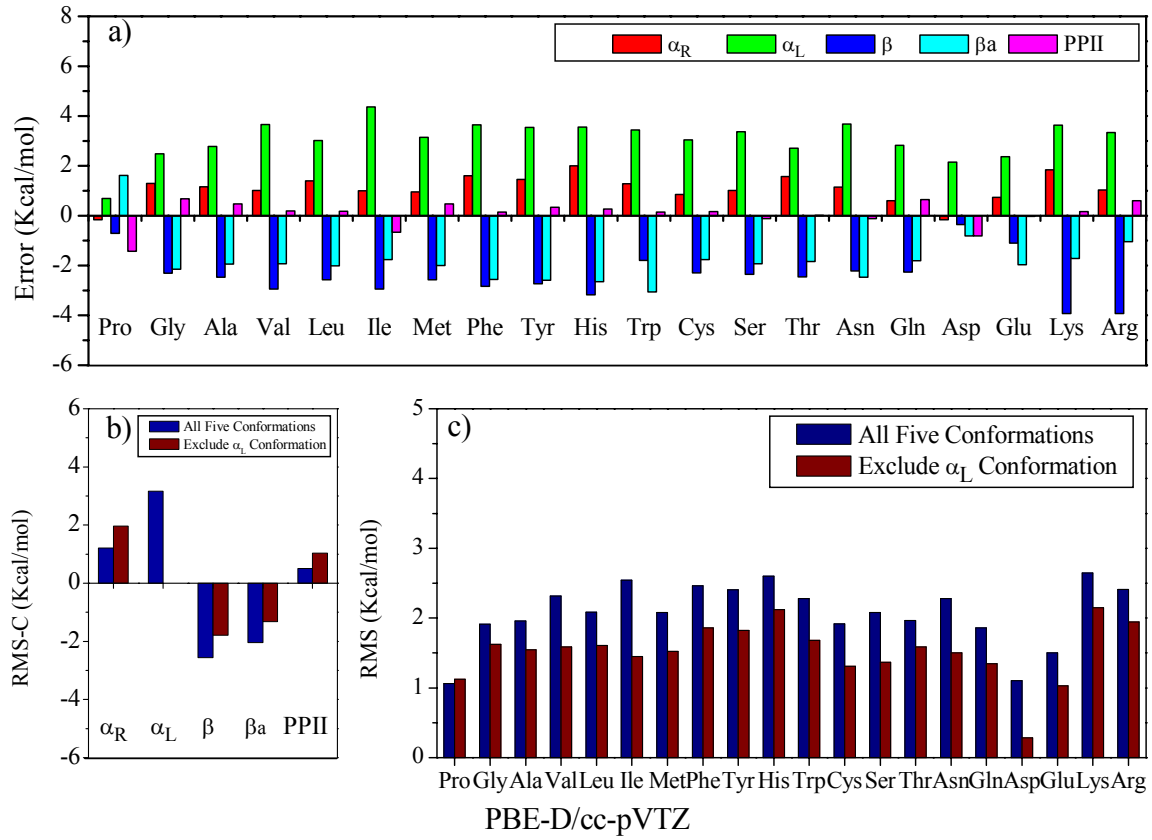

Figure S7. The performance of PBE/cc-pVTZ with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S7a – S7c show the performance of PBE/cc-pVTZ with the AMBER99 dispersion correction. After the correction, the energy of conformation PPII was overestimated and the RMS values are slightly better than the original ones.

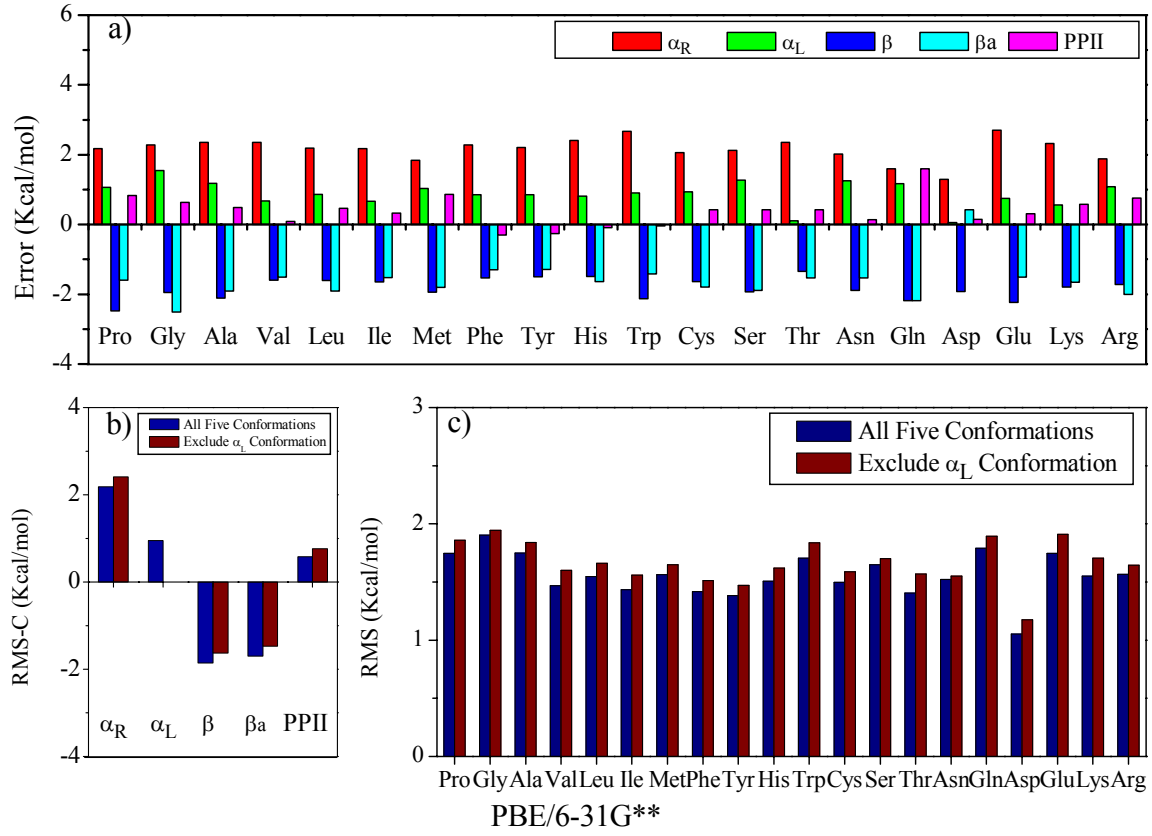

Figure S8. The performance of PBE/6-31G**. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S8a – S8c show the performance of PBE/6-31G**. First, this method overestimates conformation energies of α_R, α_L and PPII(except for Phe, Tyr, His and Trp) and underestimates the conformation energies of β, βa(except for Asp) in Fig. S8a. Second, the RMSs of the twenty amino acids all are ～ 2.0 kcal/mol and the RMS value of Asp is obviously smaller than others (Fig. S8c and Table S3d).

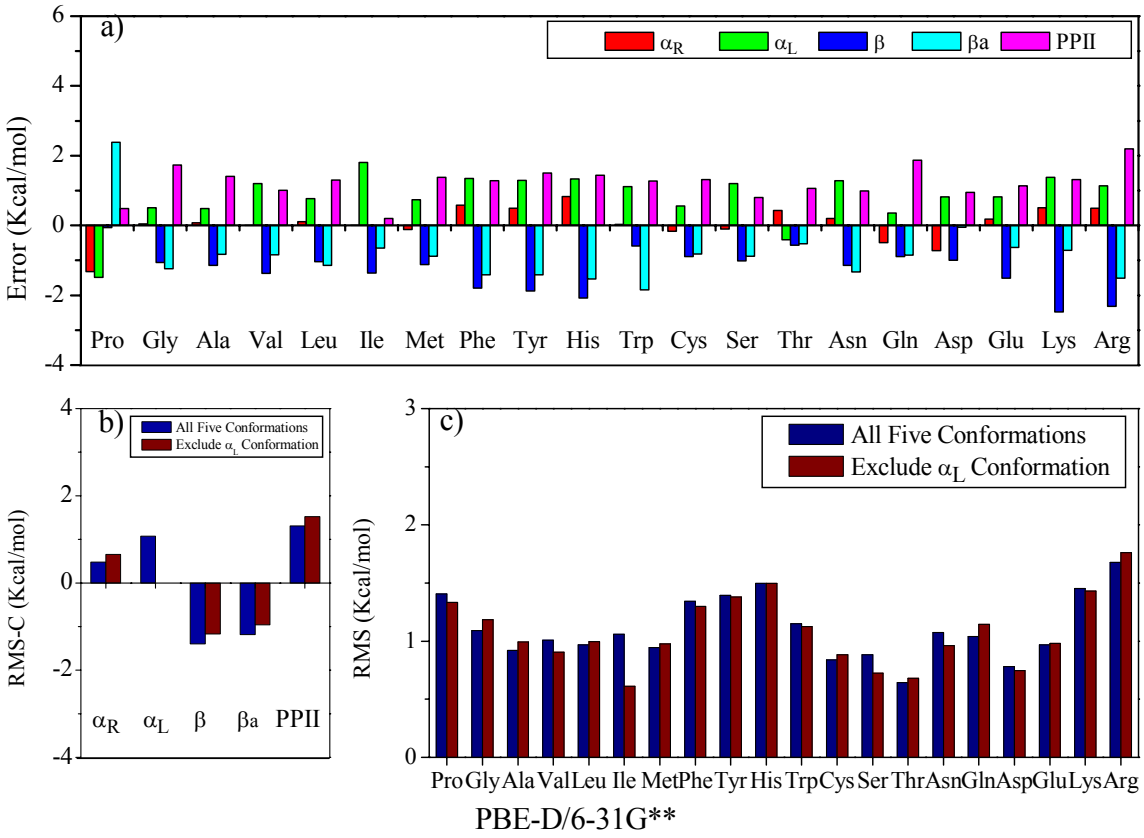

Figure S9. The performance of PBE/6-31G** with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S9a – S9c show the performance of PBE/6-31G** with the AMBER99 dispersion correction. After the correction, the RMS-C of conformation PPII was even worse than before, but the RMS values for all amino acids are slightly better than the original ones.

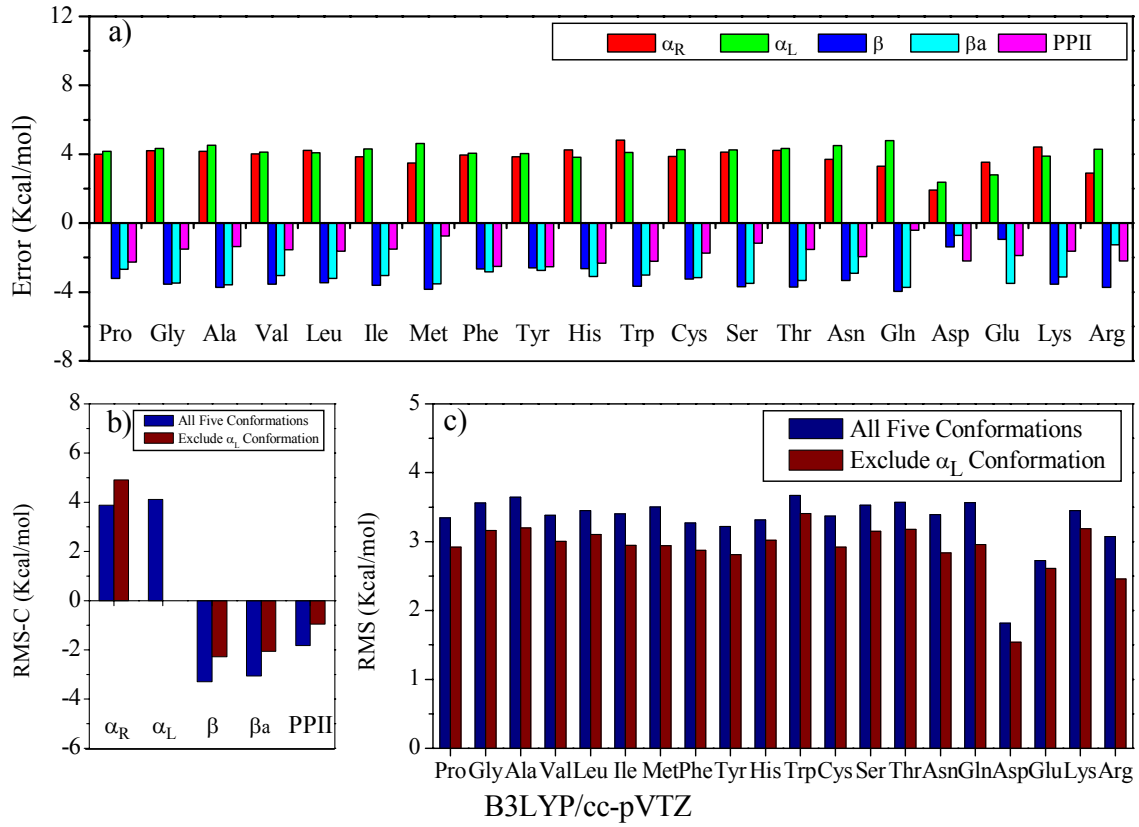

Figure S10. The performance of B3LYP/cc-pVTZ. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S10a – S10c show the performance of B3LYP/cc-pVTZ. First, this method overestimates the compact conformation energies (α_R and α_L) and underestimates the extended conformation energies (β, βa and PPII, except for the β conformations of Cys and Glu) in Fig. S10a. Thus, it appears to overestimate the short range interactions (e.g H-bond) and to underestimate the long range interactions (e.g Dispersion energy). Second, the energetic description on the compact conformation (α_R and α_L) is worse than the extended conformation by more than 1 .0 kcal/mol (Fig. S10b and Table S3c). Third, the RMSs of the twenty amino acids all are more than 3.0 kcal/mol except for Asp ang Glu(Fig. S10c and Table S3d).

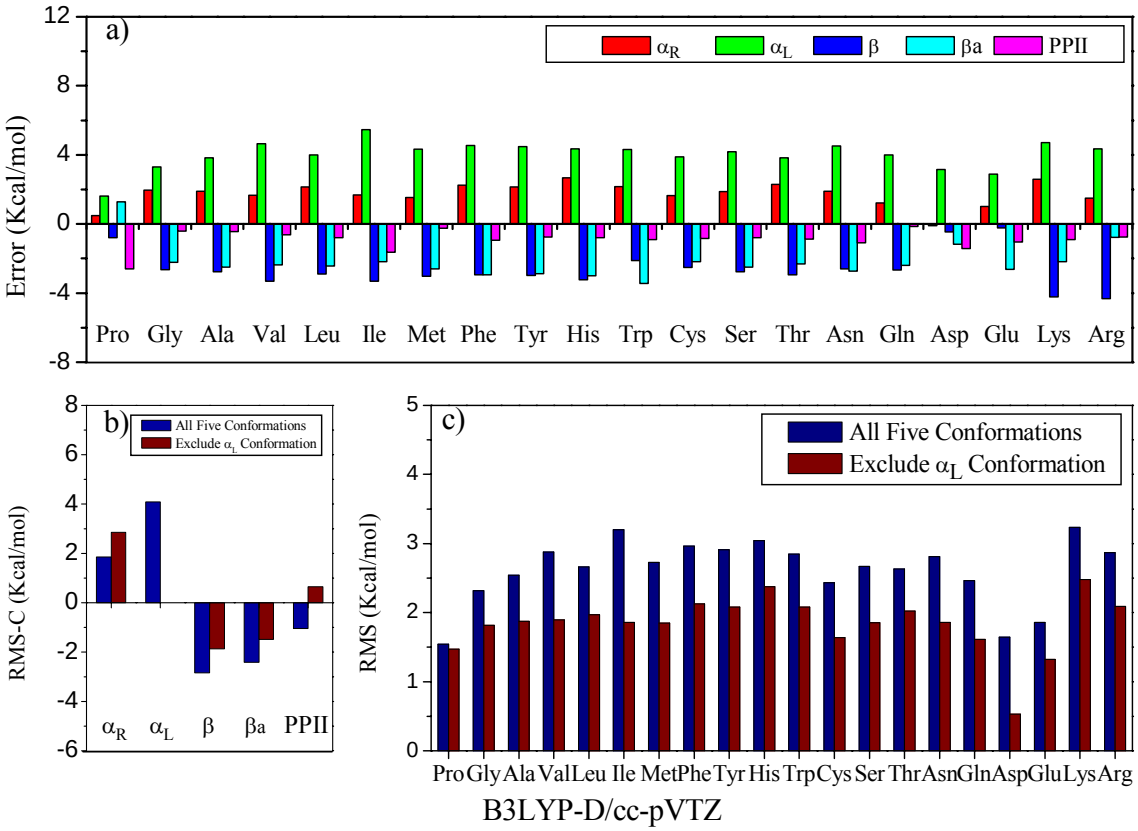

Figure S11. The performance of B3LYP/cc-pVTZ with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S11a – S11c show the performance of B3LYP/cc-pVTZ with the AMBER99 dispersion correction. After the correction, the energy of conformation α_R was overestimated and the RMS values are slightly better than the original ones.

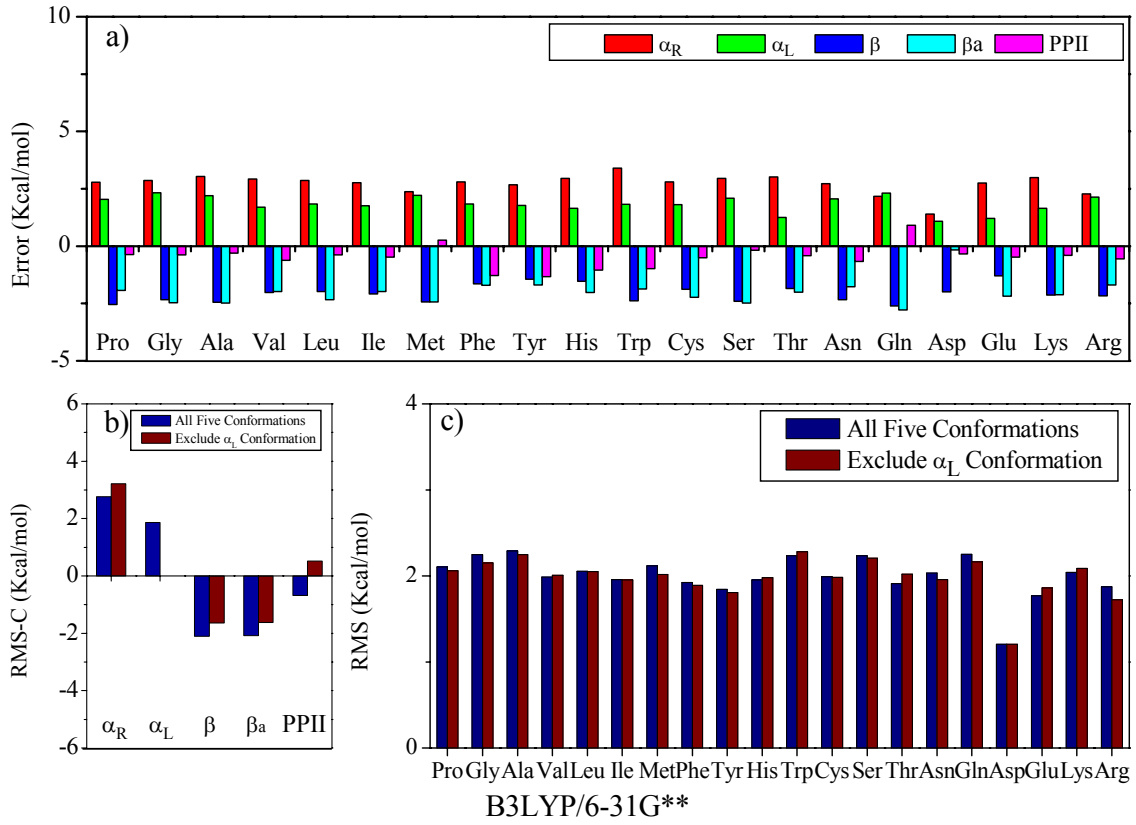

Figure S12. The performance of B3LYP/6-31G**. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S12a – S12c show the performance of B3LYP/6-31G**. First, this method overestimates the compact conformation energies (α_R and α_L) and underestimates the extended conformation energies (β, βa and PPII, except for the PPII conformations of Met and Gln) (Fig. S12a). Thus, this method appears to overestimate the short range interactions (e.g H-bond) but underestimate the long range interactions (e.g. Dispersion energy). Second, the energetic description of α_R is slightly worse than the other four conformations by ~1.0-2.0 kcal/mol (Fig. S12b and Table S3c). Third, the RMS over the twenty amino acids is ~2.0 kcal/mol except for Asp (Fig. S12c and Table S3d).

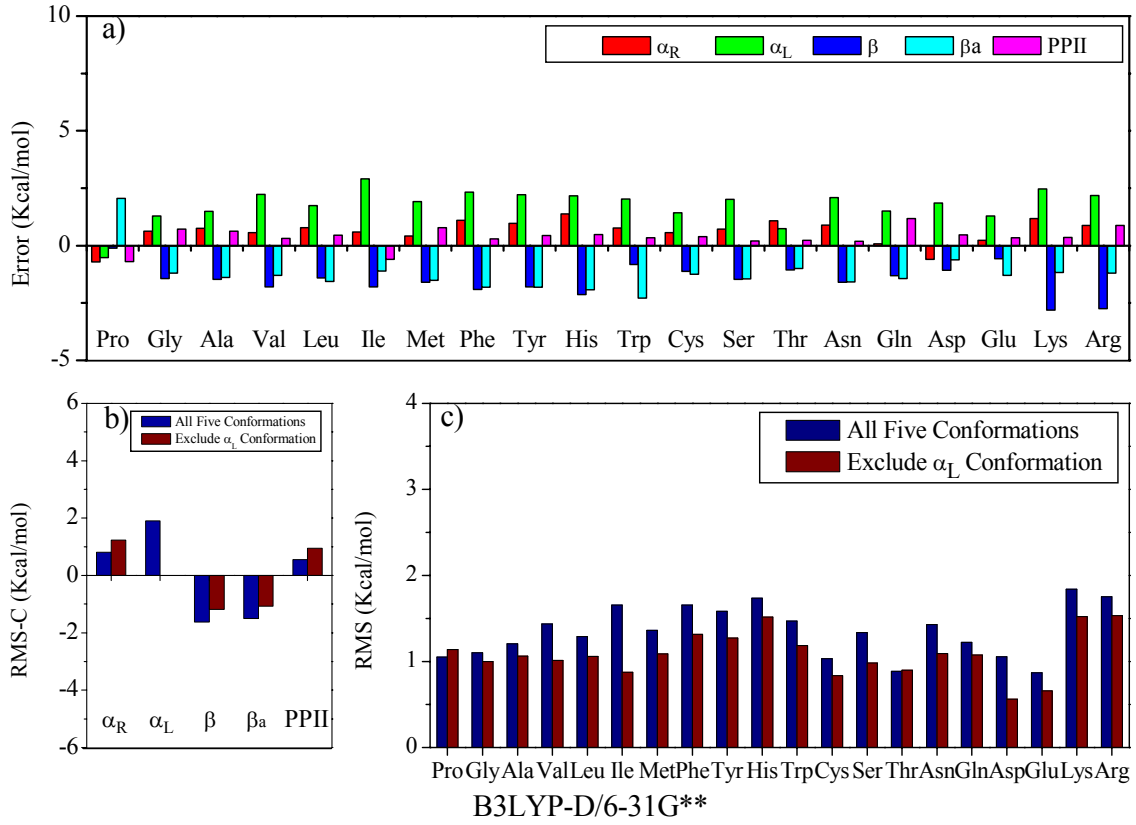

Figure S13. The performance of B3LYP/6-31G** with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S13a – S13c show the performance of B3LYP/6-31G** with the AMBER99 dispersion correction. This method overestimates energies of conformation α_R, α_L and PPII and underestimate energies of conformation β, βa. The RMS values obviously become smaller than the original ones

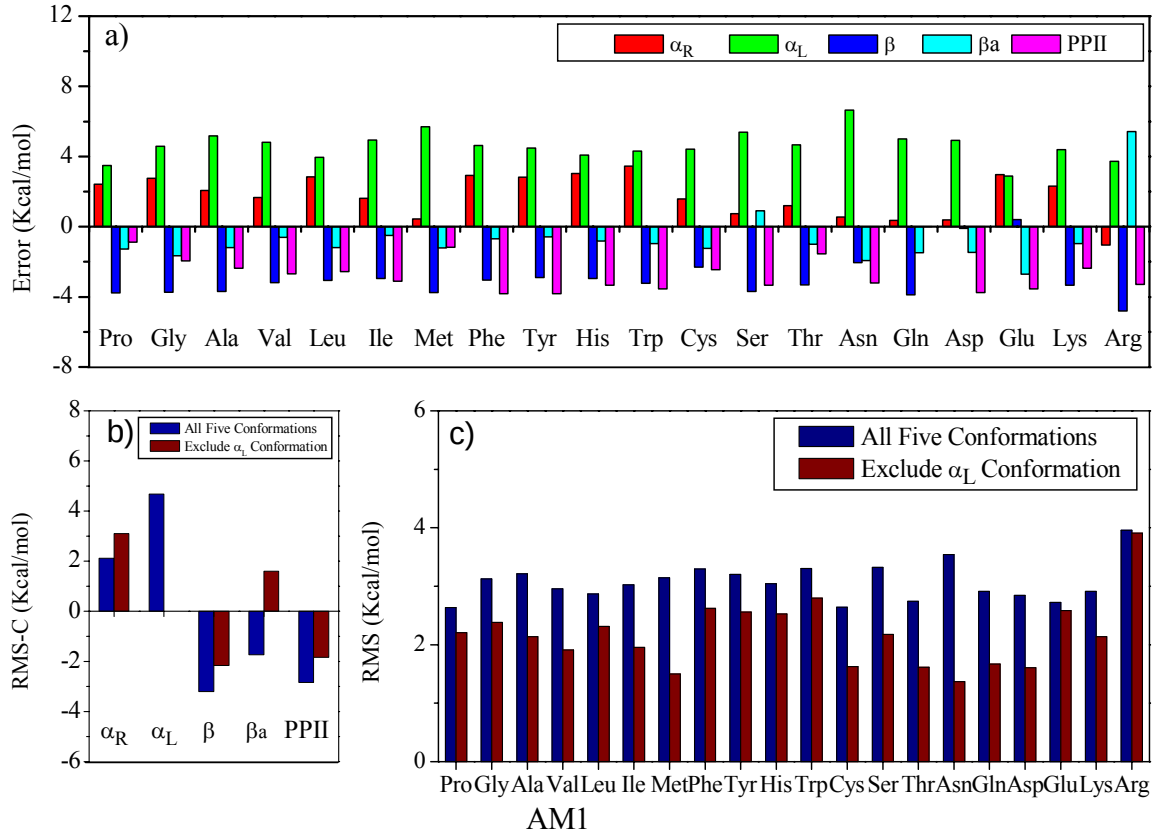

Figure S14. The performance of AM1. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S14a – S14c show the performance of AM1. First, this method overestimates the compact conformation energies (α_R and α_L, except for the α_R of Arg), but underestimates the extended conformation energies (except for the βa conformations of Ser and Arg, the β conformation of Glu) (Fig. S14a). Thus, this method appears to overestimate the short range interactions (e.g. H-bond) and underestimate the long range interactions (e.g. Dispersion energy). Second, the description for α_L (4.68 kcal/mol of RMS-C) is much worse than other conformations (2.11, -3.20, -1.74 and -2.83 kcal/mol for α_R, β, βa and PPII, respectively) in Table S3c and Fig. S14b. Third, RMS of all the amino acids are more than 2.0 kcal/mol.

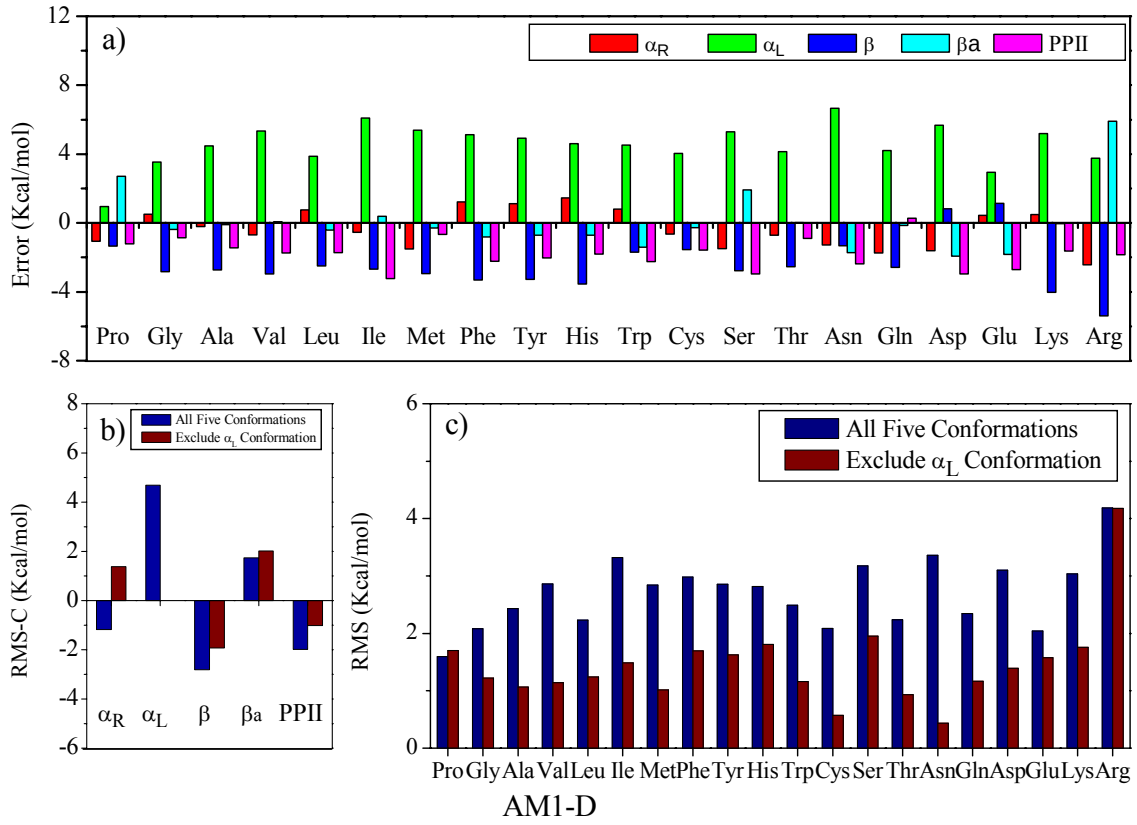

Figure S15. The performance of AM1 with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S15a – S15c show the performance of AM1 with the AMBER99 dispersion correction. With the dispersion correction, this method underestimates the energy of conformation α_R and overestimates the energy of conformation βa. The RMS values are improved after the correction except for Arg.

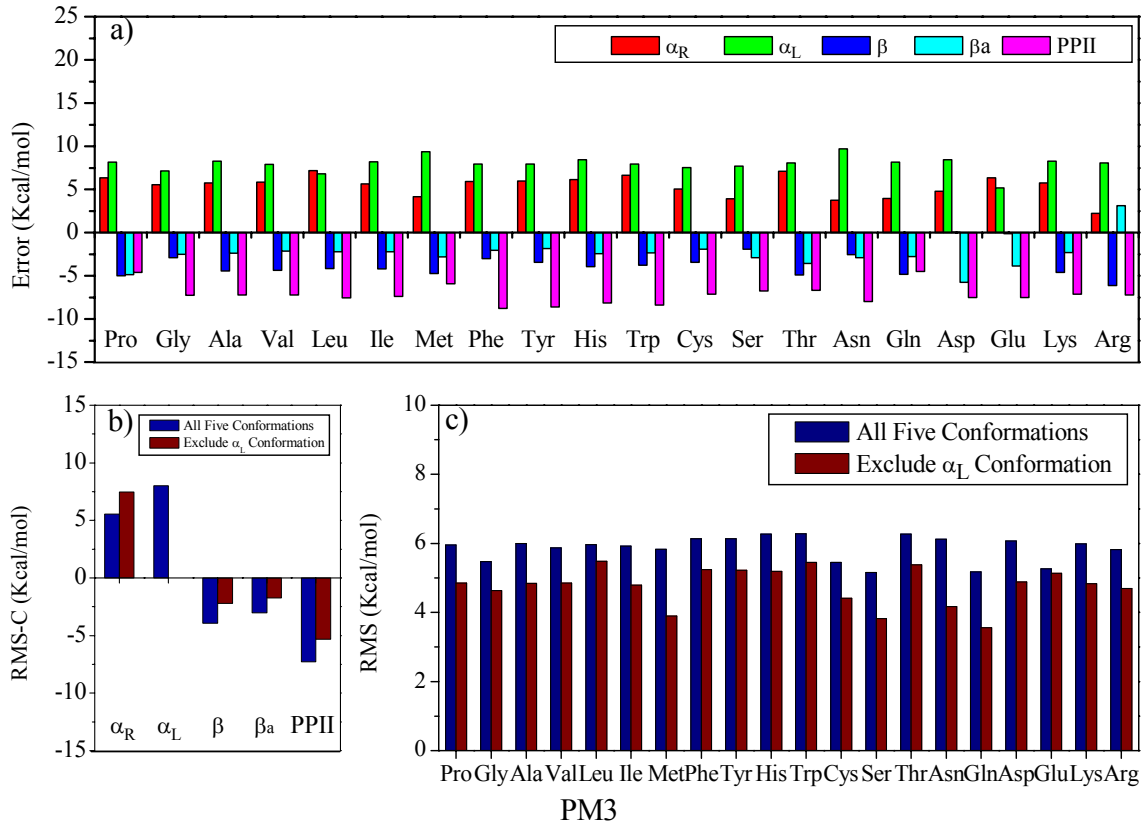

Figure S16. The performance of PM3. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S16a – S16c show the performance of PM3. First, this method overestimates the compact conformation energies (α_R and α_L), but underestimates the extended conformation energies (β, βa and PPII, except for the βa conformation of Arg.) (Fig. S16a). Thus, this method appears to significantly overestimate the short range interactions (e.g H-bond) and to significantly underestimate the long range interactions (e.g. Dispersion energy). Second, the RMS-Cs using all five conformation data are 5.54, 8.01, -3.93, -3.01 and -7.27 kcal/mol for α_R, α_L, β, βa and PPII, respectively (Table S3c and Figure S16b). These suggest a poor energetic description of all conformations except for βa. Third, the energetic description over twenty amino acids is uniformly bad (i.e. even the RMS-Nα_L is ~ 5.0 kcal/mol) in Figure S16c and Table S4d.

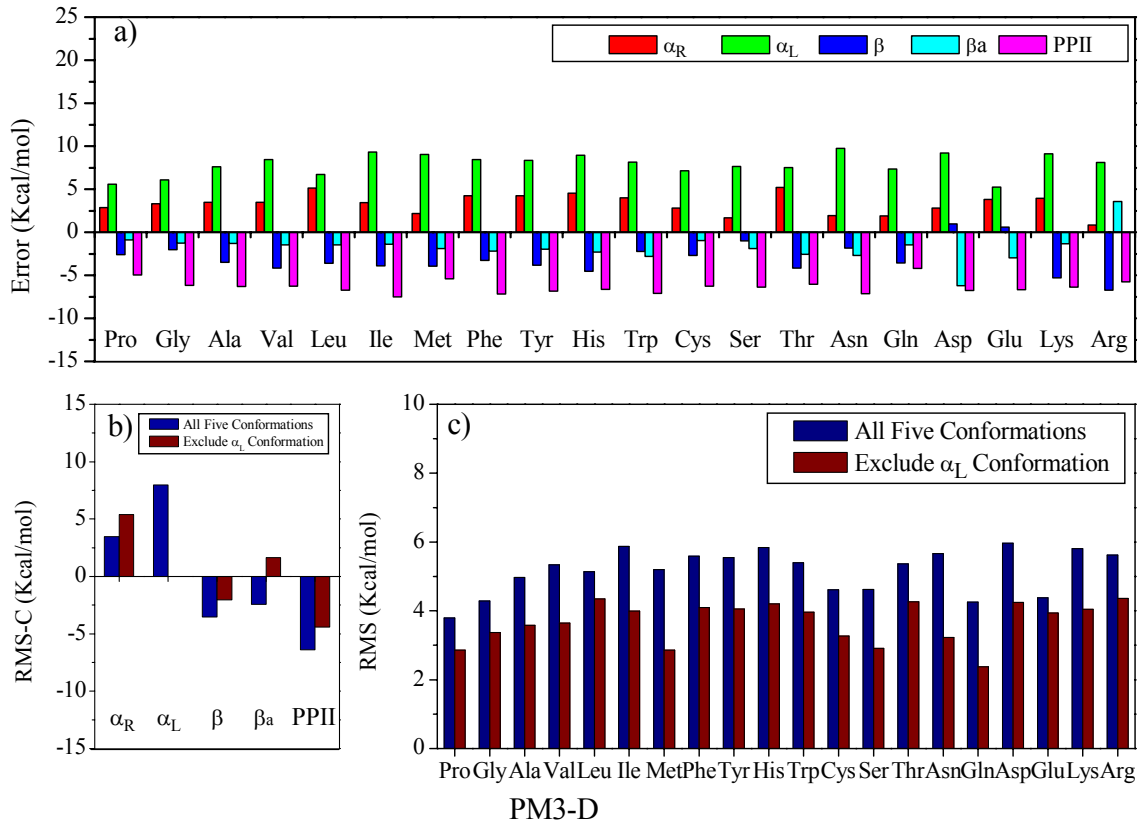

Figure S17. The performance of PM3 with the AMBER99 dispersion correction. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S17a – S17c show the performance of PM3 with the AMBER99 dispersion correction. With the dispersion correction, the RMS values are slightly improved.

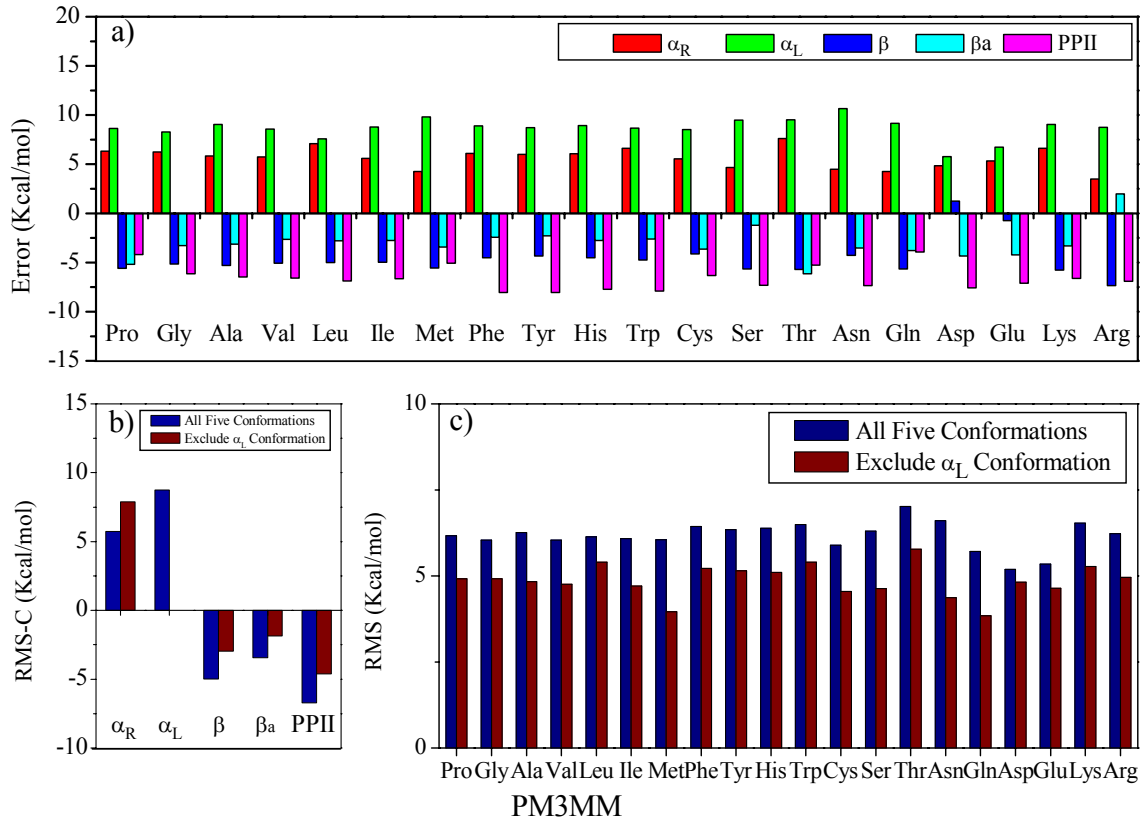

Figure S18. The performance of PM3MM. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S18a – S18c show the performance of PM3MM. First, this method overestimates the compact conformation energies (α_R and α_L) and underestimates the extended conformation energies (β (except for Asp), βa (except for Arg) and PPII) in Fig. S18a. Thus, this method appears to overestimate the short range interactions (e.g H-bond) but to underestimate the long range interactions (e.g. Dispersion). Second, the RMS-Cs using all five conformation data are 5.73, 8.74, -4.98, -3.45 and -6.71 kcal/mol for α_R, α_L, β, βa and PPII, respectively (Table S3c and Figure S18b). These suggest a poor energetic description of all conformations except for βa. Third, the energetic description over twenty amino acids is uniformly bad (i.e. even the RMS-Nα_L is ~ 5.0 kcal/mol) in Figure S18c and Table S4d.

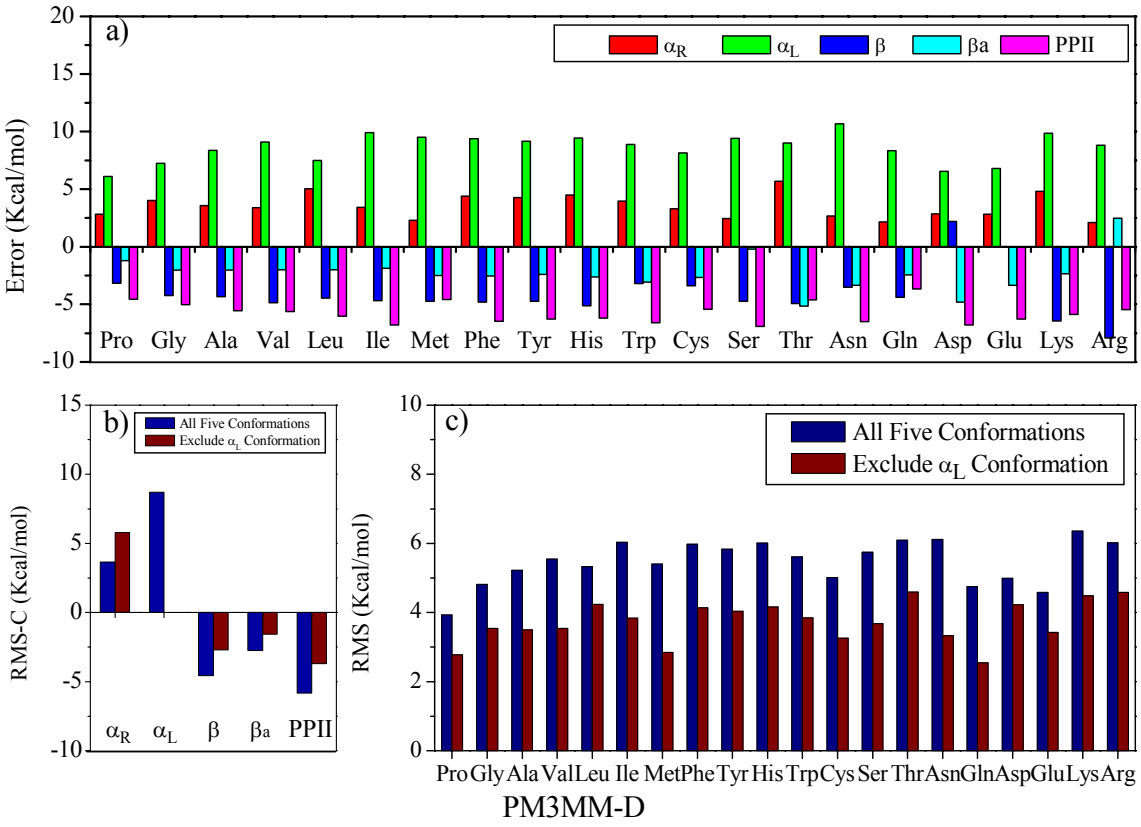

Figure S19. The performance of PM3MM with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S19a – S19c show the performance of PM3MM with the AMBER99 dispersion correction. With the dispersion correction, the RMS values are slightly improved.

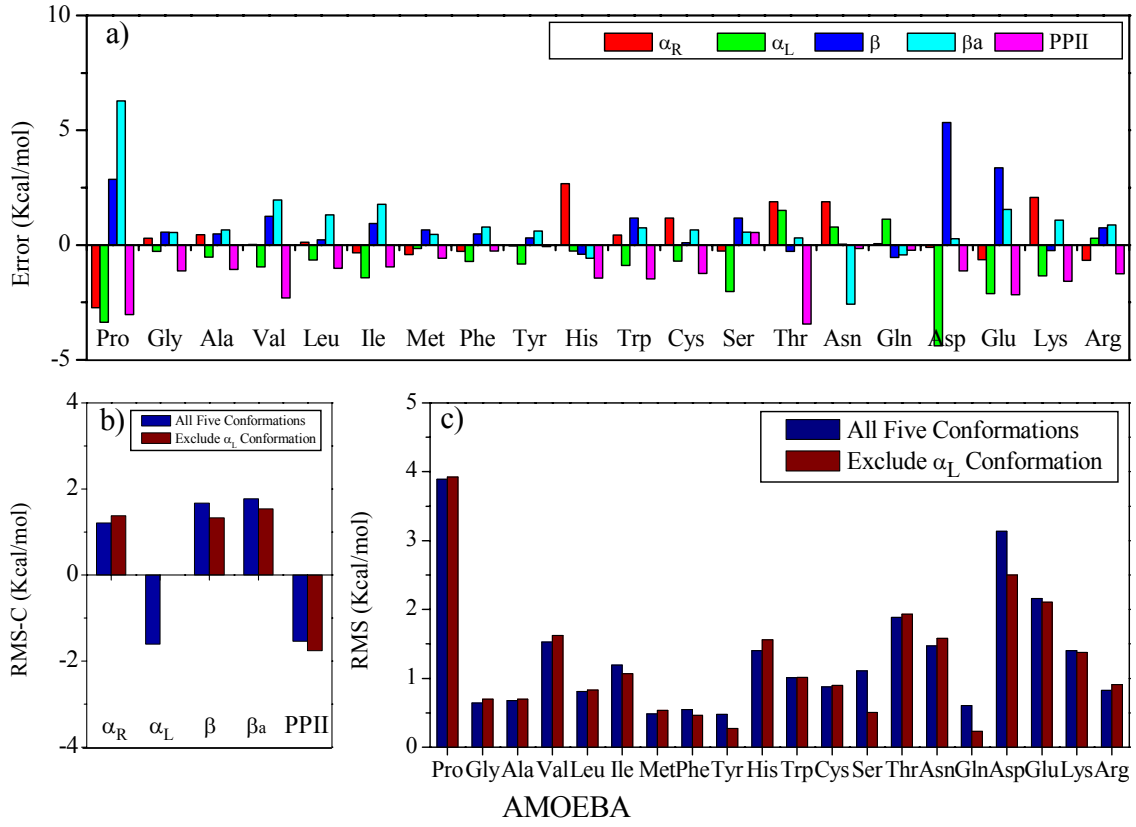

Figure S20. The performance of force field AMOEBA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S20a – S20c show the performance of AMOEBA. First, this method slightly underestimates the energies of conformations PPII (except for Ser) and α_L (except for Thr, Asn, Gln), but overestimates the energies of β (except for His, Thr, Gln and Lys) and βa (except for His, Asn and Gln). As to α_R, it overestimates the energies of nine amino acids but underestimates the other eleven amino acids. Second, the RMS-Cs of five conformations is all ~1.5 kcal/mol, indicating a reasonable description on conformation energy (Figure S20b and Table S3c). Third, energetic descriptions for some amino acids are very good (e.g. Met, Phe, Tyr and Gln, their RMS is ranged from 0.5 to 0.6 kcal/mol), but they are very bad for some amino acids (e.g. 3.89, 3.13 and 2.16 kcal/mol of RMS for Pro, Asp and Glu respectively).

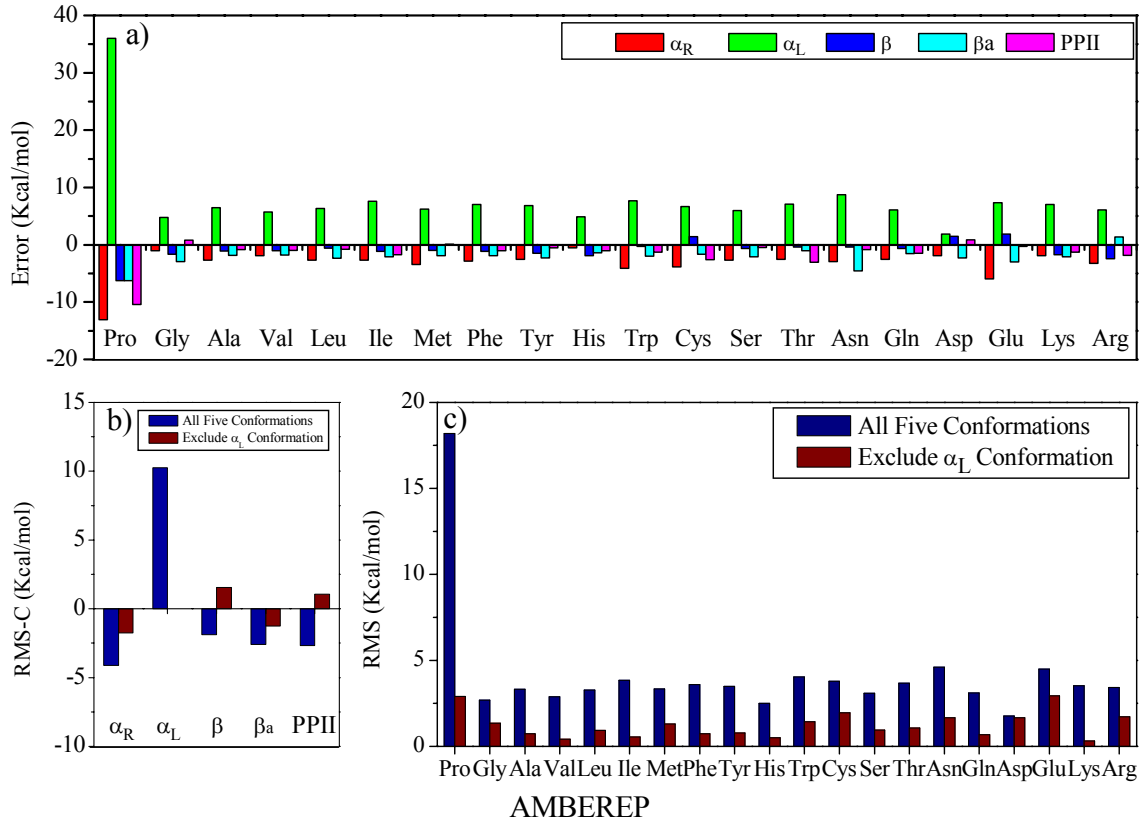

Figure S21. The performance of force field AMBEREP. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S21a – S21c show the performance of force field AMBEREP. First, this method overestimates the energies of conformations α_L (especially for Pro, up to 36.00 Kcal/mol), but underestimates the energies of other conformations (except for βa conformations of Pro and Arg, β conformations of Cys and Asp and Glu, PPII conformations of Gly and Asp). Second, the RMS-C calculations show the bad descriptions of α_L conformations (Figure S21b and Table S3c). Third, the energetic description for Pro is obviously worse than other amino acids (Figure S21c, Table S3d and Table S4d).

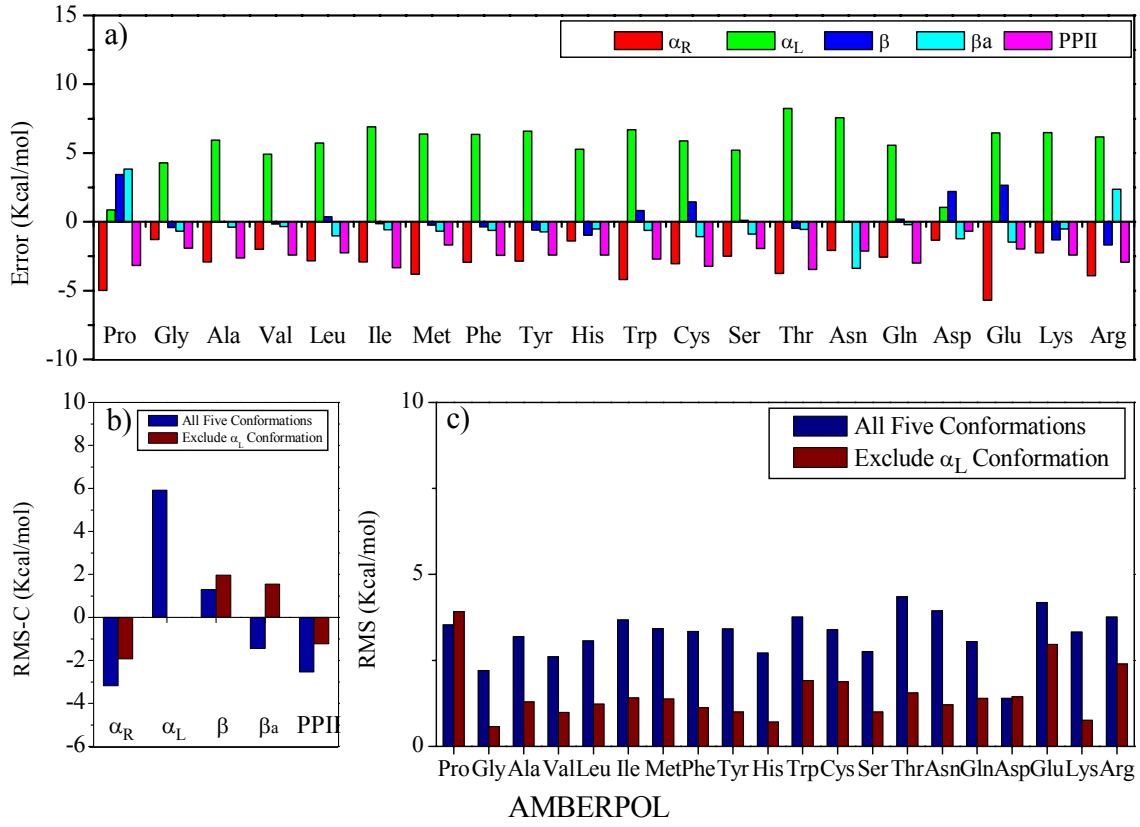

Figure S22. The performance of force field AMBERPOL. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S22a – S22c show the performance of force field AMBERPOL. First, this method overestimates the energies of conformations α_L. But underestimate the energies of other four conformations (except for β conformations of Pro, Leu, Trp, Cys, Gln, Asp, Glu, and βa conformations of Pro and Arg.

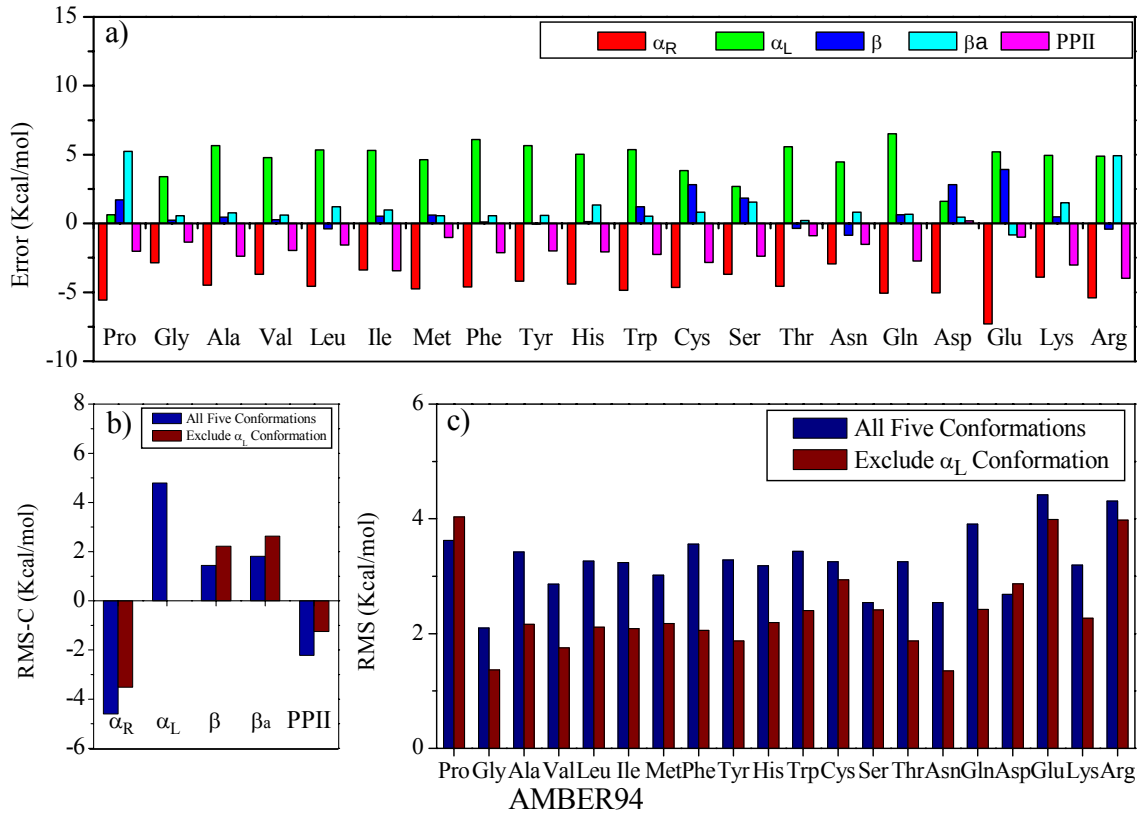

Figure S23. The performance of AMBER94. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S23a – S23c show the performance of force field AMBER94. First, this method underestimates the energies of conformations α_R and PPII, it overestimates the energies of α_L, βa (except for Glu) and β (except for Leu, Thr, Asn and Arg) in Fig. S23a. Second, Energetic description for conformations α_R and α_L are worse than the other three conformations by ~2.0 kcal/mol (Figure S23b and Table S3c). Third, when α_L conformation is excluded, the energetic descriptions for some amino acids (e.g. Pro, Glu and Arg) are worse than the others by over 1 kcal/mol of RMS-Nα_L (Figure S23c and Table S4d).

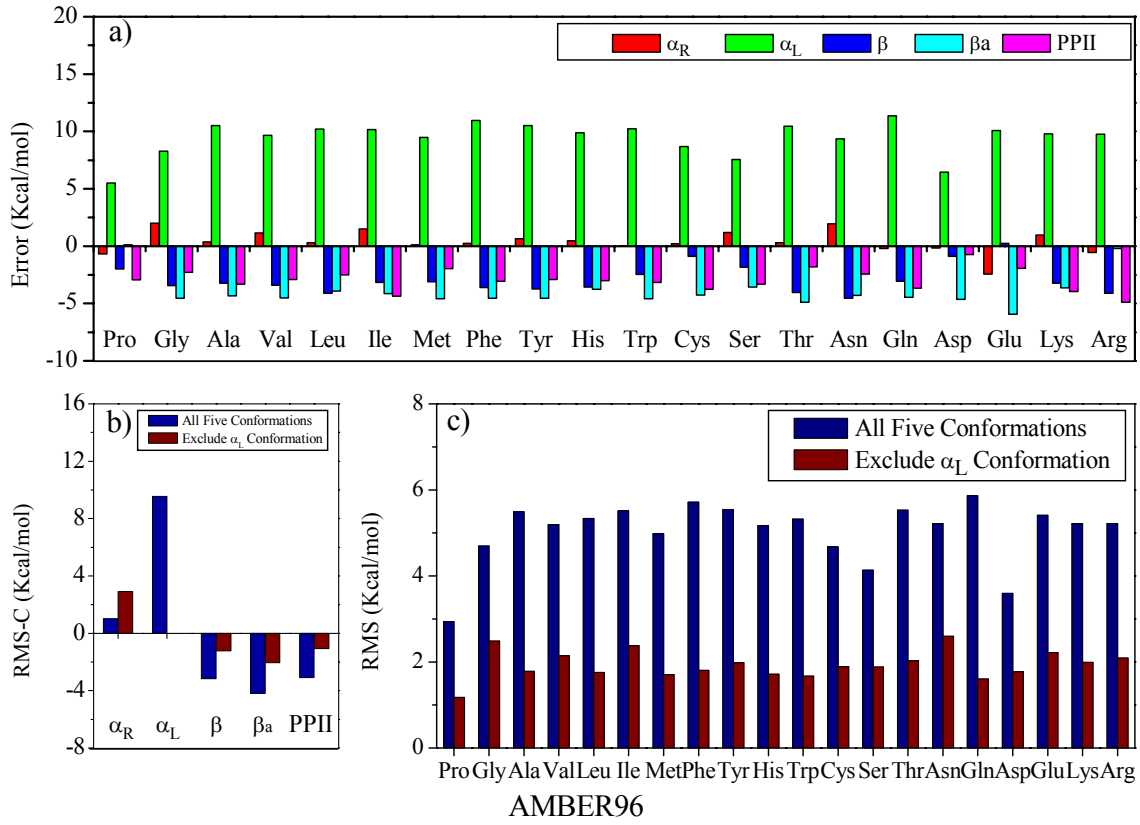

Figure S24. The performance of force field AMBER96. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S24a – S24c show the performance of force field AMBER96. This method overestimates the energies of conformations α_L and α_R (except for Pro, Gln, Asp and Arg), and underestimates the energies of PPII, βa and β (except for Glu). Energy description for conformation α_L over all amino acids (RMS-C for α_L is 9.55 kcal/mol) is much worse than the other three conformations (Figure S24b and Table S3c). RMS-Nα_L for all amino acids is about 1.93 kcal/mol when α_L conformation is excluded (Figure S24c and Table S4d).

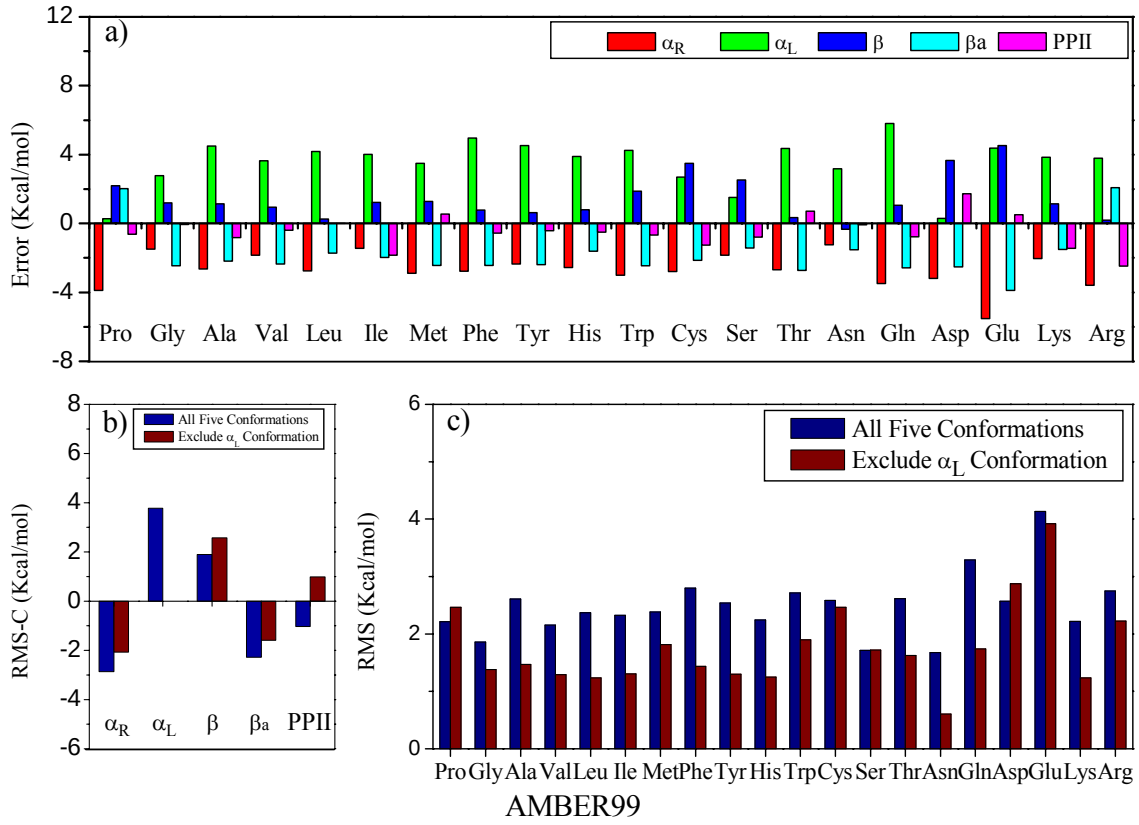

Figure S25. The performance of force field AMBER99. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S25a – S25c show the performance of force field AMBER99. First, this method overestimates the energies of conformations β (except for Asn) and α_L, but underestimates the conformation energies of PPII (except for Met, Thr, Asp and Glu), βa (except for Pro and Arg) and α_R. Second, the energetic description for conformation α_L over all amino acids (RMS-C for α_L is 3.78 kcal/mol) is much worse than the other conformations by more than 1 kcal/mol in magnitude (Figure S25b and Table S3c). Third, the energetic descriptions for residues Pro, Cys, Asp and Glu are significantly worse than the others, even when α_L conformation is excluded (Figure S25c and Table S4d).

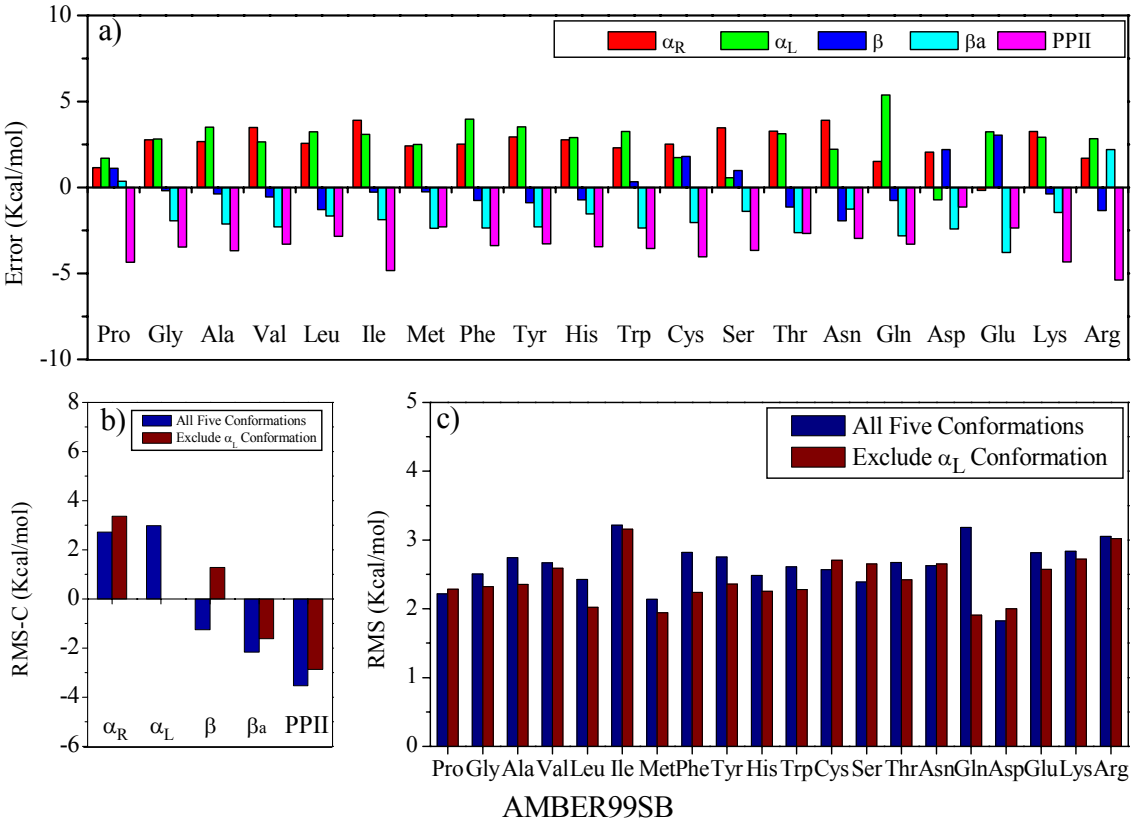

Figure S26. The performance of force field AMBER99SB. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S26a – S26c show the performance of force field AMBER99SB. This method overestimates the energies of the compact conformations and underestimates those of the extended conformations (β except for Pro, Cys, Ser, Asp and Glu, βa except for Pro and Arg) (Fig. S26a).

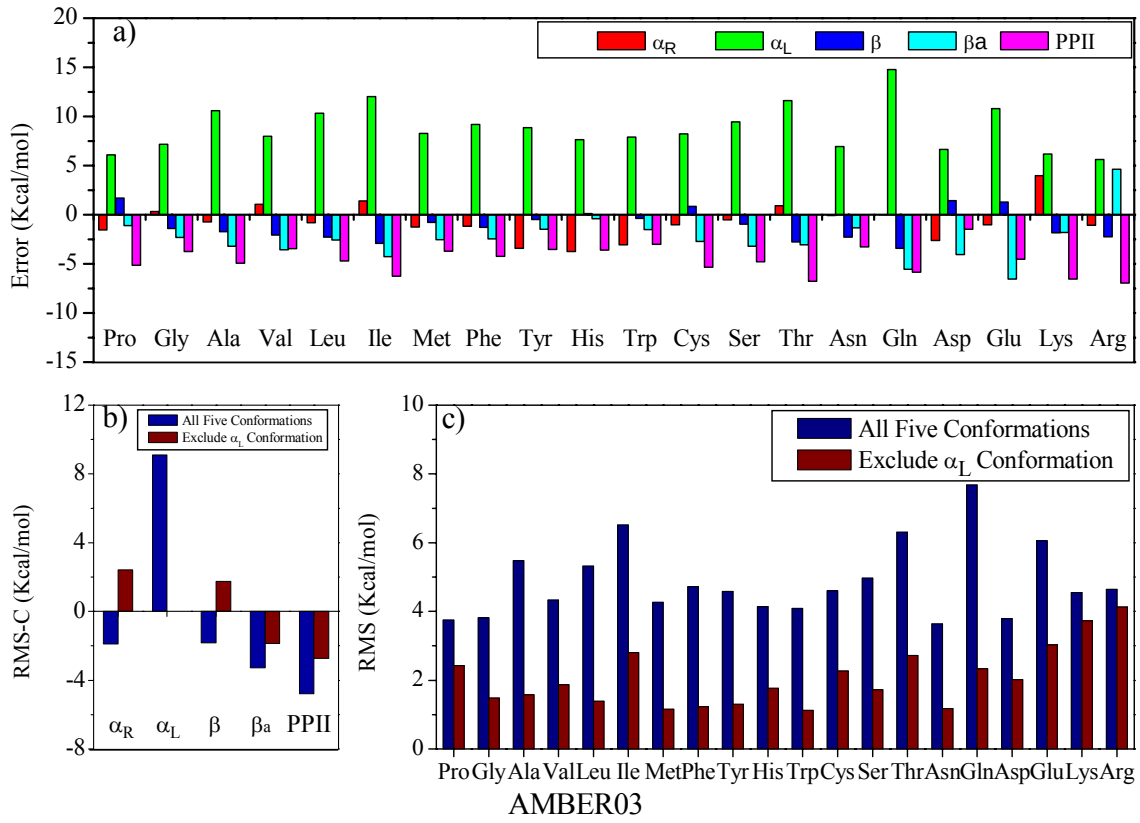

Figure S27. The performance of force field AMBER03. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S27a – S27c show the performance of force field AMBER03. First, this method largely overestimates the energies of conformation α_L, but underestimates the energies of conformations α_R (except for Gly, Val, Ile, Thr and Lys), β (except for Pro, Cys, Asp and Glu), βa (except for Arg) and PPII. Second, the overall energetic descriptions for α_L (9.10 kcal/mol of RMS-C) are worse than α_R, β, βa and PPII (-1.89, -1.82, -3.28 and -4.79 kcal/mol of RMS-C) (Figure S27b and Table S3c).

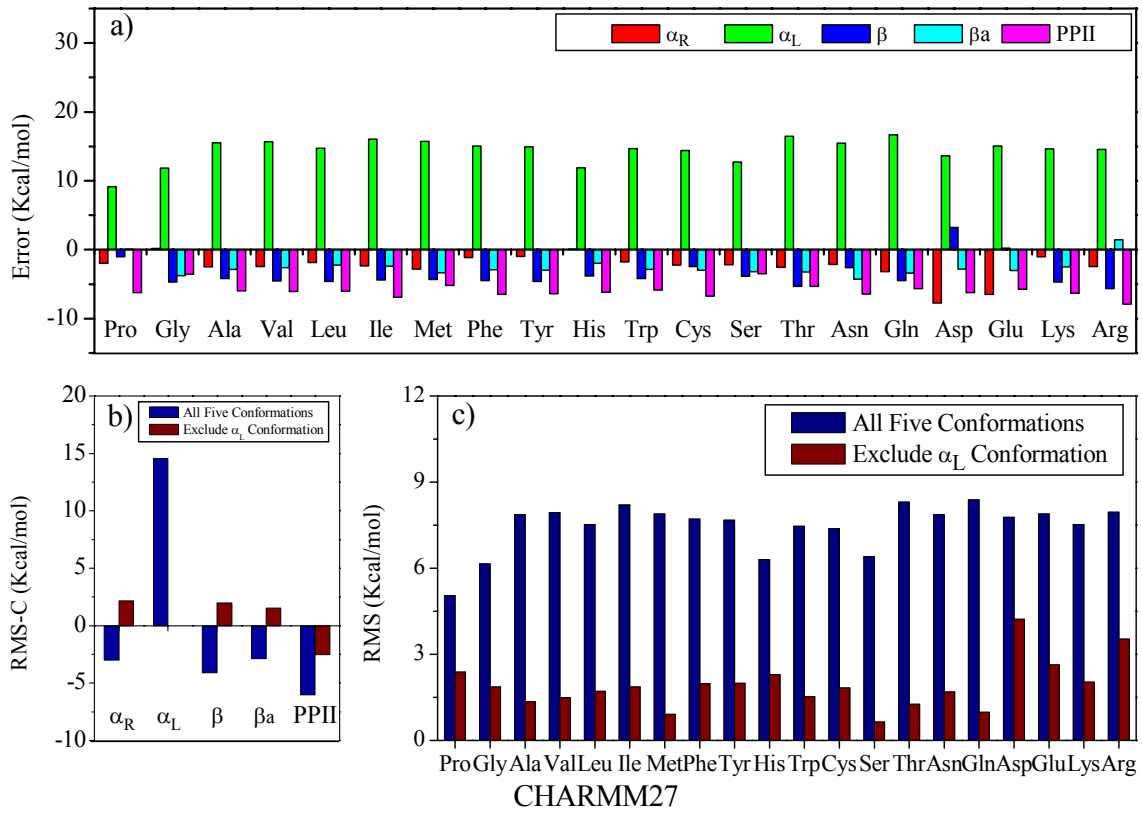

Figure S28. The performance of force field CHARMM27. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S28a – S28c show the performance of force field CHARMM27. First, this method largely overestimates the energies of conformation α_L, but underestimates the energies of conformations α_R (except for Gly), β (except for Asp and Glu), βa (except for Arg) and PPII. Second, the overall descriptions for α_L and PPII (14.55 and -6.02 kcal/mol of RMS-C) are worse than α_R, β and βa (-2.99, -4.10 and -2.87 kcal/mol of RMS-C) (Figure S28b and Table S3c). Third, after excluding α_L, energetic descriptions for some amino acids (e.g. ASP and Arg) are still worse than the others by over 1.0 kcal/mol (Fig. S28c and Table S4d).

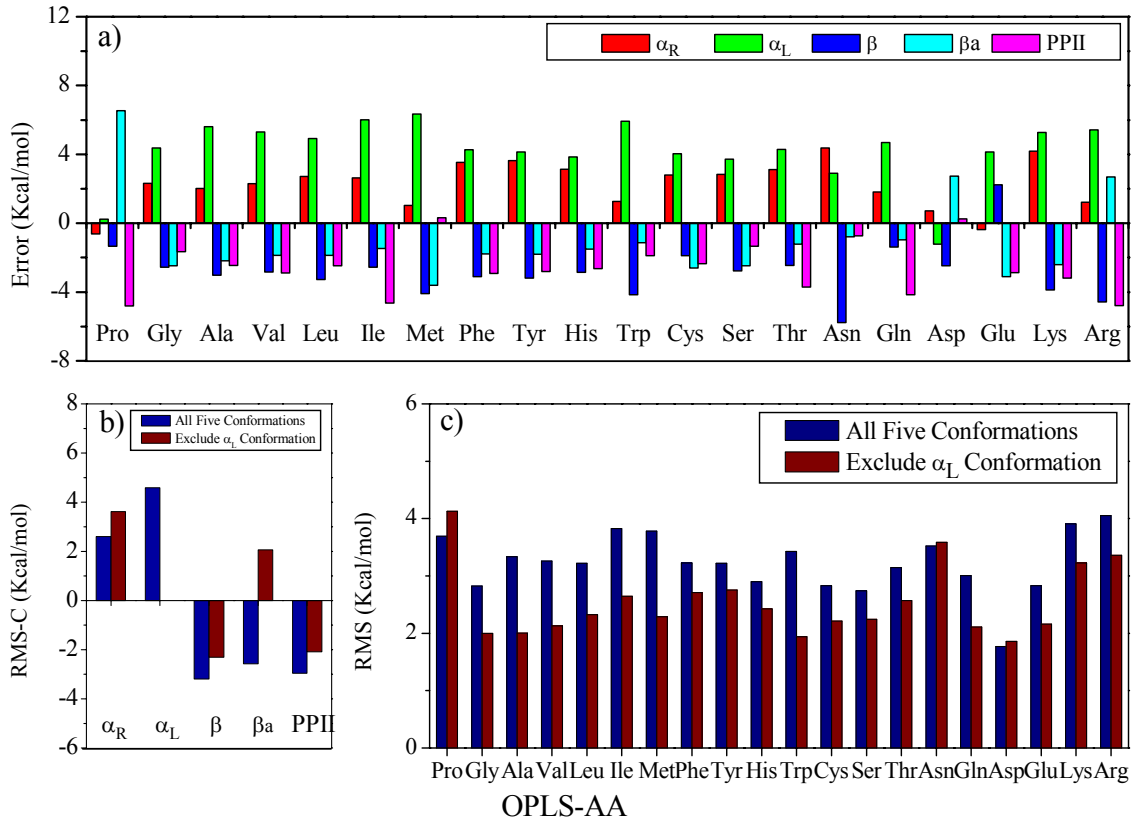

Figure S29. The performance of force field OPLS-AA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S29a – S29c show the performance of force field OPLS-AA. First, this method overestimates the energies of conformations α_L (except for Asp) and α_R (except for Pro and Glu), but it underestimates the energies of conformations βa (except for Pro, Asp and Arg), β (except for Glu) and PPII. Second, the energetic description for conformation α_L over all amino acids (4.58 kcal/mol of RMS-C) is worse than the other conformations by over 1.0 kcal/mol (Figure S29b and Table S3c). Third, after excluding α_L, the energetic descriptions for some amino acids (e.g. Pro, Asn, Cys and Arg) are still worse than the others by over 1.0 kcal/mol.

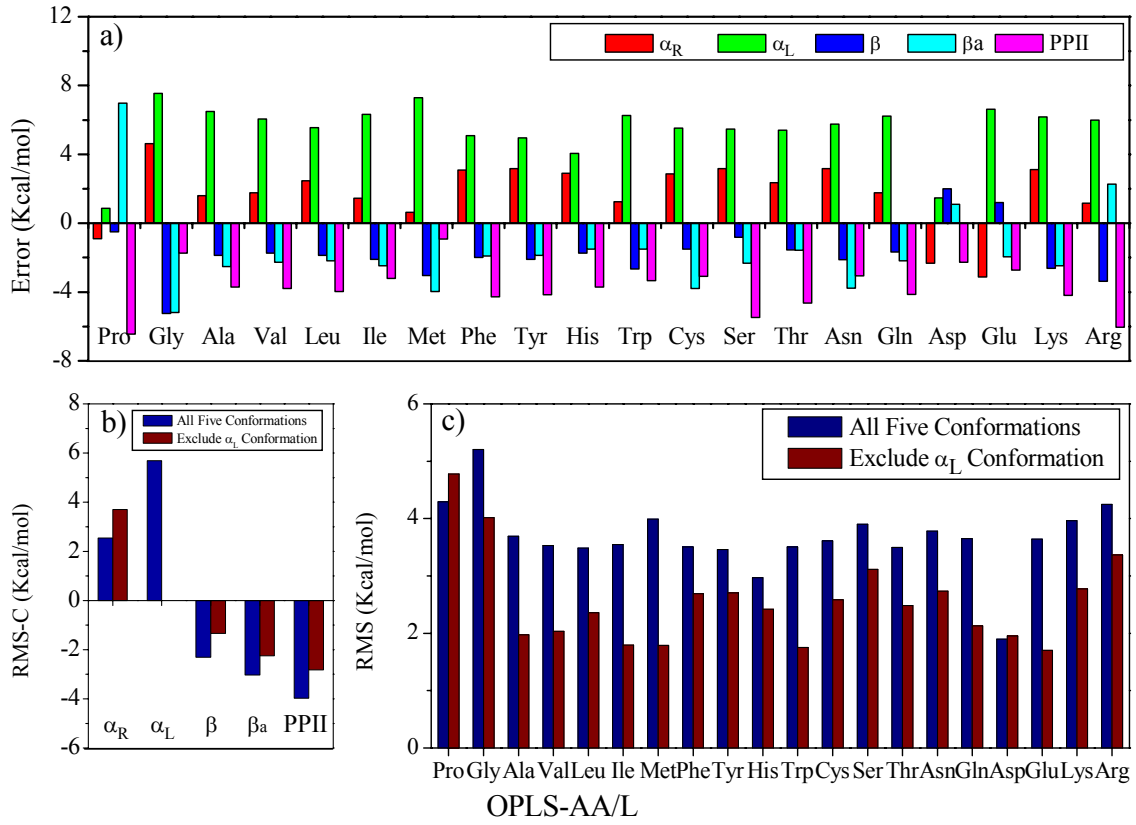

Figure S30. The performance of force field OPLS-AA/L. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S30a – S30c show the performance of force field OPLS-AA/L. First, this method overestimates the energies of conformations α_R (except for Pro, Asp and Glu) and α_L, but it underestimates the energies of conformations βa (except for Pro, Asp and Arg), β (except for Asp and Glu) and PPII. Second, the energetic descriptions for conformation α_L and PPII over all amino acids (their RMS-Cs are 5.70 and -3.97 kcal/mol) are worse than the other conformations (Figure S30b and Table S3c). Third, after excluding α_L, energy descriptions for some amino acids (e.g. Pro, Asn and Arg) are still worse than the others.

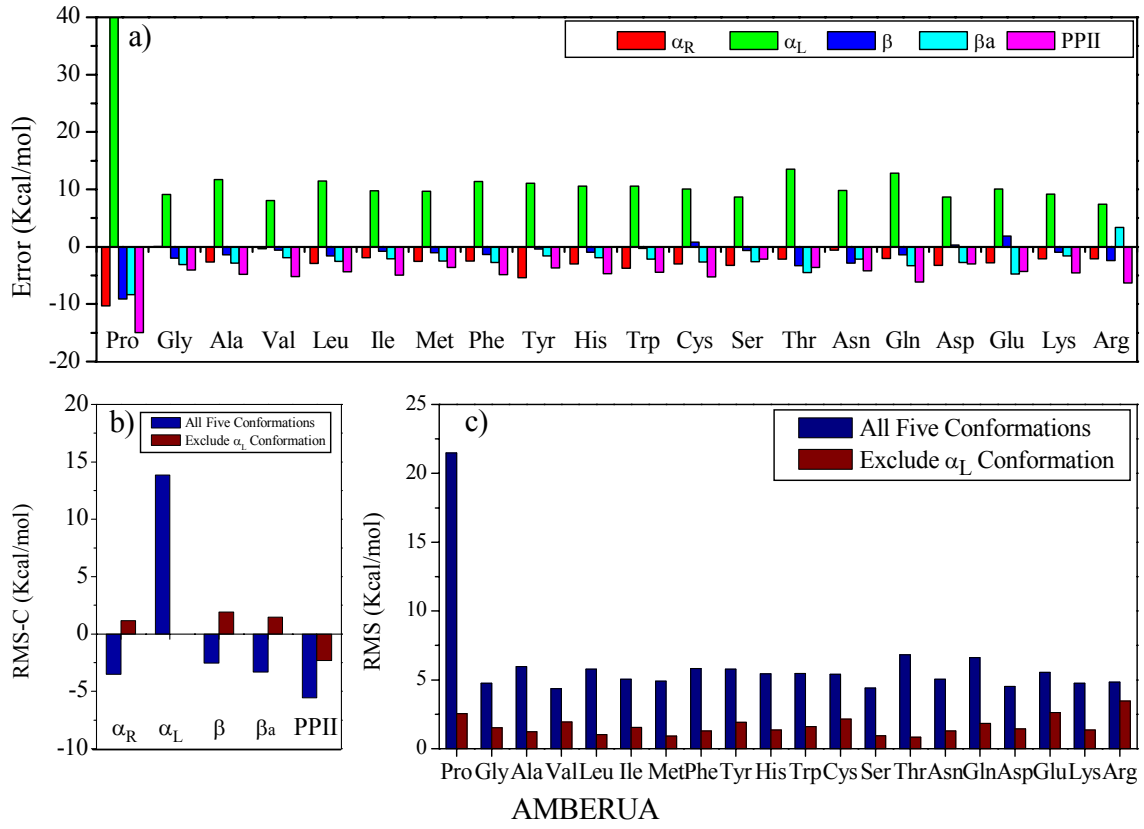

Figure S31. The performance of force field AMBERUA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S31a – S31c show the performance of force field AMBERUA. First, this method overestimates the energies of conformations α_L, especially for Pro, 42.71 Kcal/mol. But underestimate the energies of other conformations (except for β conformations of Cys, Asp and Glu). Second, the RMS-C calculations show the bad descriptions of α_L conformations (Figure S31b and Table S3c). Third, the energetic description for Pro is obviously worse than other amino acids (Figure S31c, Table S3d and Table S4d).

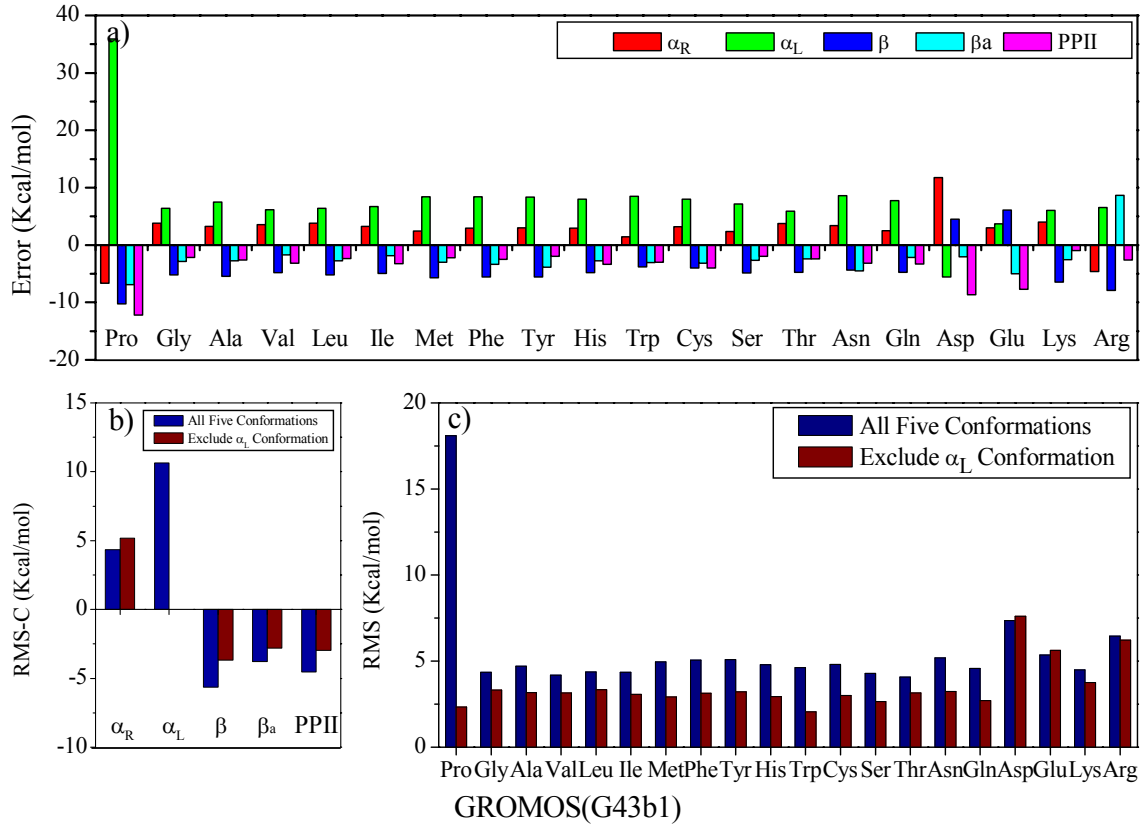

Figure S32. The performance of force field GROMOS(G43b1). a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S32a – S32c show the performance of force field GROMOS(G43b1). This method overestimates the energies of conformations α_R (except for Pro, Arg) and α_L (except for Asp), but it underestimates the energies of conformations βa (except for Arg), β (except for Asp and Glu) and PPII.

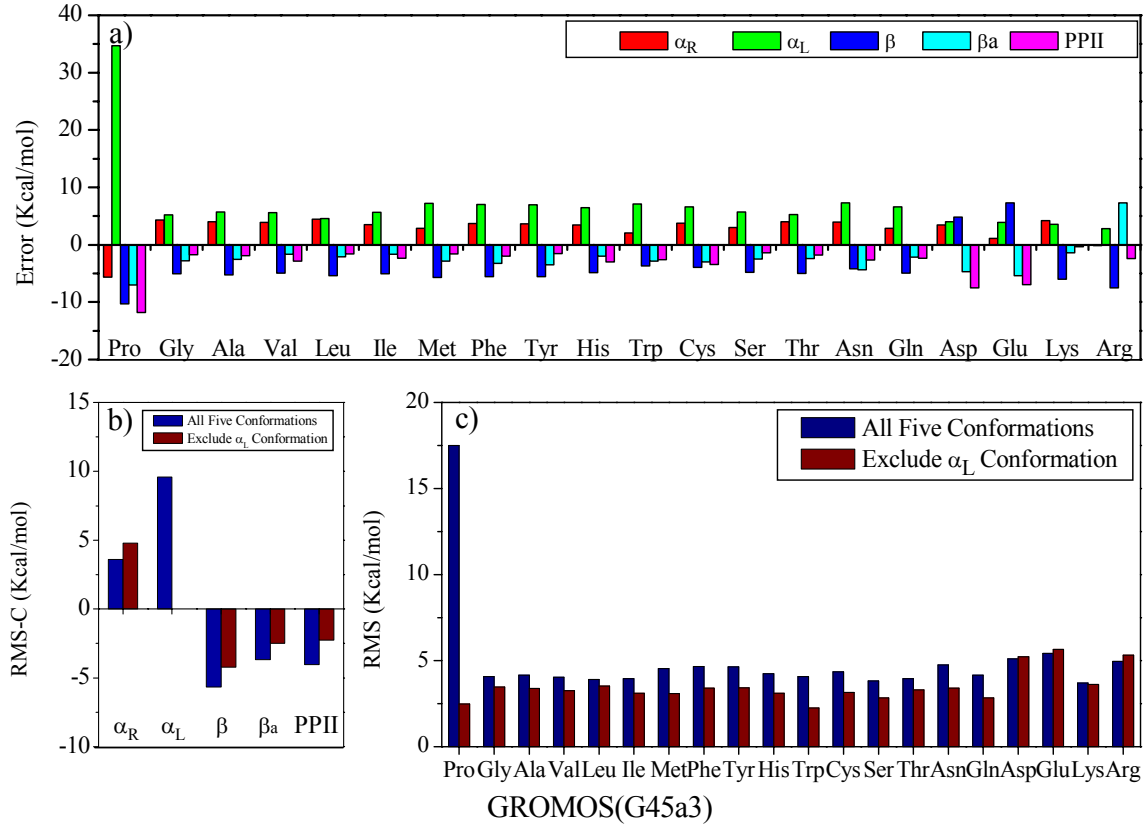

Figure S33. The performance of force field GROMOS(G45a3). a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S33a – S33c show the performance of force field GROMOS(G45a3). This method overestimates the energies of conformations α_R (except for Pro) and α_L, but it underestimates the energies of conformations βa (except for Arg), β (except for Asp and Glu) and PPII.

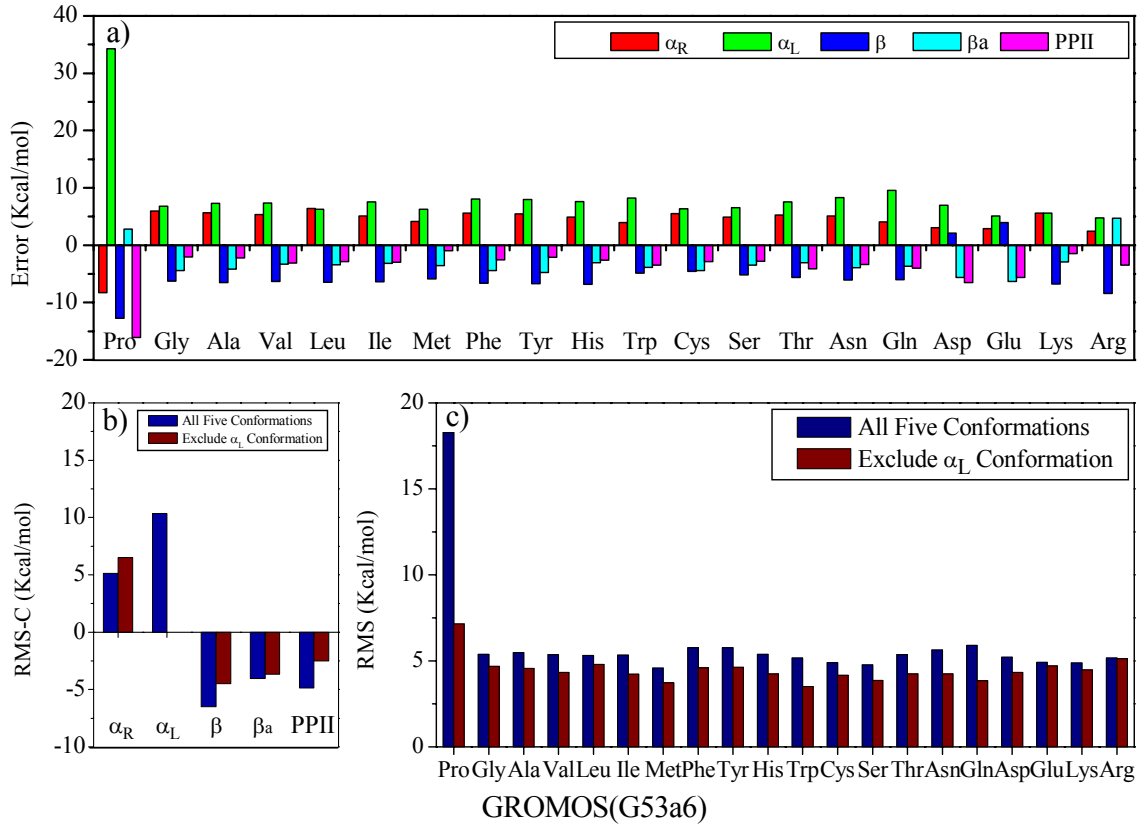

Figure S34. The performance of force field GROMOS(G53a6). a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

Figures S34a – S34c show the performance of force field GROMOS(G53a6). Τηισ μετηοδ οωερεστιματεσ τηε ενεργιεσ οφ χονφορματιονσ α_R (except for Pro) and α_L, but it underestimates the energies of conformations βa (except for Pro and Arg), β (except for Asp and Glu) and PPII.

Supporting Information B. Using MP2/cc-pVTZ//M05-2X/6-31G results as the "true" value.**

Table S1. Relative energies (with reference to the α_R conformation) calculated by MP2/cc-pVTZ//M05-2X/6-31G** methods for five conformations of each tetrapeptide (kcal/mol).

	α_R	α_L	β	β_a	PPII
Pro	0.00	2.28	4.71	5.90	2.36
Gly	0.00	1.49	4.13	1.79	3.22
Ala	0.00	2.24	3.91	1.81	3.27
Val	0.00	3.42	2.56	0.51	3.38
Leu	0.00	3.10	3.72	1.16	3.39
Ile	0.00	3.93	2.40	0.56	2.63
Met	0.00	-0.40	3.44	1.52	1.71
Phe	0.00	-0.71	0.26	-1.68	3.22
Tyr	0.00	-0.53	-0.58	-2.34	3.06
His	0.00	0.07	1.02	-0.18	2.89
Trp	0.00	0.06	2.95	-0.80	3.15
Cys	0.00	0.87	4.22	1.48	4.47
Ser	0.00	1.19	4.63	1.56	3.95
Thr	0.00	1.97	5.91	4.64	4.43
Asn	0.00	-0.90	1.74	1.81	3.92
Gln	0.00	1.81	3.01	0.77	-1.56
Asp	0.00	16.45	0.15	7.40	13.26
Glu	0.00	4.91	-0.23	3.09	7.38
Lys	0.00	2.82	4.02	0.83	1.15
Arg	0.00	-4.10	-1.00	-18.16	-4.61

Table S2a. Energy offset (E_c) (kcal/mol) of each tetrapetpide obtained from Eq. 2 in minimizing RMS of each method over 5 conformations.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg
M05-2X/cc-pVTZ	1.46	1.51	1.58	1.34	1.33	1.34	1.25	1.47	1.31	1.45	2.07	1.36	1.48	1.27	1.35	1.14	0.56	0.92	1.45	1.32
M05-2X-D[a]/cc-pVTZ	-2.04	-0.73	-0.69	-1.01	-0.75	-0.83	-0.70	-0.23	-0.40	-0.12	-0.57	-0.87	-0.75	-0.65	-0.47	-0.96	-1.46	-1.61	-0.37	-0.07
M05-2X/6-31G**	0.55	0.47	0.69	0.60	0.35	0.56	0.37	0.71	0.68	0.60	0.97	0.56	0.59	0.48	0.60	0.24	0.52	0.65	0.38	0.84
M05-2X-D[a]/6-31G**	-2.95	-1.76	-1.59	-1.75	-1.73	-1.60	-1.59	-0.99	-1.03	-0.97	-1.67	-1.67	-1.64	-1.45	-1.22	-1.86	-1.49	-1.87	-1.43	-0.56
PBE/cc-pVTZ	3.68	3.69	3.77	3.52	3.66	3.36	3.10	3.19	2.78	3.57	4.10	3.71	3.52	3.75	3.17	2.83	2.05	3.33	3.89	2.59
PBE-D[a]/cc-pVTZ	0.18	1.46	1.49	1.17	1.58	1.19	1.14	1.48	1.07	2.00	1.46	1.48	1.29	1.83	1.35	0.74	0.04	0.80	2.07	1.20
PBE/6-31G**	2.52	2.45	2.69	2.50	2.38	2.37	2.02	2.16	1.83	2.41	2.85	2.68	2.39	2.61	2.22	1.73	1.50	2.77	2.56	2.06
PBE-D[a]/6-31G**	-0.98	0.21	0.41	0.15	0.30	0.20	0.07	0.46	0.12	0.83	0.21	0.45	0.16	0.69	0.40	-0.37	-0.52	0.25	0.74	0.67
B3LYP/cc-pVTZ	4.32	4.37	4.50	4.17	4.41	4.04	3.68	3.84	3.48	4.25	4.98	4.50	4.38	4.48	3.91	3.44	2.11	3.60	4.65	3.08
B3LYP-D[a]/cc-pVTZ	0.83	2.13	2.23	1.81	2.33	1.88	1.72	2.14	1.77	2.68	2.34	2.27	2.15	2.56	2.09	1.34	0.10	1.08	2.83	1.69
B3LYP/6-31G**	3.12	3.03	3.36	3.07	3.05	2.96	2.57	2.68	2.31	2.96	3.57	3.41	3.22	3.27	2.92	2.30	1.61	2.82	3.22	2.45
B3LYP-D[a]/6-31G**	-0.38	0.79	1.09	0.72	0.97	0.79	0.61	0.98	0.60	1.39	0.93	1.18	0.99	1.35	1.10	0.20	-0.41	0.29	1.41	1.06
AM1	2.76	2.92	2.40	1.81	3.03	1.82	0.63	2.80	2.45	3.03	3.63	2.20	1.01	1.46	0.74	0.48	0.60	3.03	2.54	-0.86
AM1-D[a]	-0.73	0.68	0.12	-0.55	0.95	-0.35	-1.33	1.10	0.74	1.46	0.99	-0.03	-1.22	-0.46	-1.08	-1.61	-1.42	0.51	0.72	-2.25
PM3	6.69	5.72	6.10	5.98	7.39	5.82	4.33	5.81	5.58	6.12	6.80	5.65	4.17	7.37	3.96	4.10	5.01	6.43	5.99	2.40
PM3-D[a]	3.20	3.49	3.82	3.62	5.31	3.66	2.37	4.10	3.87	4.54	4.16	3.42	1.94	5.45	2.14	2.00	3.00	3.91	4.17	1.01
PM3MM	6.65	6.42	6.18	5.89	7.30	5.79	4.44	5.99	5.61	6.06	6.78	6.16	4.94	7.87	4.69	4.38	5.07	5.41	6.86	3.66
PM3MM-D[a]	3.15	4.19	3.90	3.54	5.22	3.62	2.49	4.29	3.90	4.49	4.14	3.93	2.71	5.95	2.87	2.28	3.06	2.89	5.05	2.27
AMOEBA	-2.40	0.45	0.78	0.18	0.31	-0.14	-0.22	-0.40	-0.41	2.68	0.61	1.80	0.02	2.14	2.08	0.19	0.11	-0.57	2.32	-0.48
AMBEREP	-12.74	-0.87	-2.37	-1.76	-2.47	-2.45	-3.24	-3.00	-2.92	-0.54	-3.97	-3.22	-2.42	-2.31	-2.73	-2.40	-1.74	-5.89	-1.70	-3.04
AMBERPOL	-4.65	-1.12	-2.58	-1.84	-2.63	-2.70	-3.62	-3.07	-3.22	-1.37	-4.01	-2.43	-2.23	-3.51	-1.87	-2.43	-1.14	-5.62	-2.01	-3.74
AMBER94	-5.22	-2.69	-4.16	-3.55	-4.38	-3.17	-4.56	-4.74	-4.58	-4.40	-4.67	-4.03	-3.42	-4.31	-2.74	-4.94	-4.84	-7.24	-3.66	-5.22
AMBER96	-0.35	2.17	0.71	1.32	0.49	1.69	0.30	0.13	0.28	0.47	0.19	0.84	1.45	0.55	2.13	-0.07	0.03	-2.37	1.21	-0.35
AMBER99	-3.54	-1.31	-2.31	-1.68	-2.55	-1.25	-2.70	-2.88	-2.73	-2.55	-2.82	-2.18	-1.58	-2.43	-1.03	-3.36	-2.99	-5.46	-1.80	-3.41
AMBER99SB	1.50	2.94	3.00	3.64	2.75	4.10	2.59	2.40	2.56	2.79	2.48	3.14	3.74	3.53	4.11	1.64	2.26	-0.11	3.50	1.88
AMBER03	-1.22	0.49	-0.41	1.23	-0.61	1.61	-1.07	-1.29	-3.81	-3.75	-2.86	-0.42	-0.25	1.19	0.12	0.15	-2.39	-0.95	4.20	-0.87
CHARMM27	-1.62	0.35	-2.18	-2.31	-1.68	-2.16	-2.64	-1.24	-1.36	0.05	-1.57	-1.64	-1.89	-2.28	-1.91	-3.04	-7.56	-6.42	-0.82	-2.26
OPLS-AA	-0.28	2.47	2.36	2.45	2.90	2.83	1.22	3.42	3.27	3.14	1.44	3.41	3.11	3.37	4.58	1.94	0.92	-0.31	4.43	1.41
OPLS-AA/L	-0.57	4.79	1.92	1.92	2.65	1.65	0.81	2.96	2.81	2.91	1.42	3.48	3.44	2.62	3.38	1.90	-2.12	-3.06	3.35	1.33
AMBERUA	-9.93	0.21	-2.34	-0.17	-2.73	-1.71	-2.35	-2.59	-5.73	-3.01	-3.54	-2.38	-2.98	-1.91	-0.40	-1.89	-3.02	-2.75	-1.86	-1.92
GROMOS(G43b1)	-6.29	3.97	3.59	3.71	4.04	3.47	2.62	2.84	2.66	2.93	1.57	3.79	2.67	3.99	3.59	2.61	12.00	3.04	4.23	-4.46
GROMOS(G45a3)	-5.27	4.50	4.33	4.02	4.64	3.70	3.07	3.57	3.26	3.45	2.24	4.39	3.25	4.26	4.17	2.99	3.64	1.21	4.43	0.06
GROMOS(G53a6)	-7.93	6.14	5.95	5.49	6.59	5.25	4.32	5.44	5.11	4.89	4.15	6.16	5.16	5.54	5.26	4.23	3.25	2.96	5.82	2.62

[a] AMBER99 dispersion correction.

Table S2b. Signed error ($error = E_{ai} - E_{bi} + E_c$, kcal/mol) using the MP2 energy as the true value

M05-2X/cc-pVTZ//M05-2X/6-31G**						M05-2X-D[a]/cc-pVTZ//M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	1.46	1.41	-0.66	-0.89	-1.32	Pro	-2.04	-1.14	1.76	3.09	-1.66
Gly	1.51	1.17	-0.65	-1.22	-0.81	Gly	-0.73	0.14	0.25	0.05	0.29
Ala	1.58	1.03	-0.57	-1.12	-0.92	Ala	-0.69	0.33	0.40	-0.04	0.00
Val	1.34	1.07	-0.51	-1.00	-0.90	Val	-1.01	1.61	-0.29	-0.34	0.03
Leu	1.33	0.97	-0.44	-1.01	-0.85	Leu	-0.75	0.87	0.12	-0.24	0.00
Ile	1.34	1.03	-0.50	-1.01	-0.85	Ile	-0.83	2.18	-0.22	-0.15	-0.98
Met	1.25	0.90	-0.56	-1.09	-0.49	Met	-0.70	0.59	0.26	-0.17	0.02
Phe	1.47	0.25	-0.08	-0.12	-1.52	Phe	-0.23	0.75	-0.35	-0.23	0.07
Tyr	1.31	0.21	-0.06	0.11	-1.58	Tyr	-0.40	0.65	-0.43	-0.01	0.18
His	1.45	0.22	-0.09	-0.25	-1.32	His	-0.12	0.74	-0.69	-0.14	0.21
Trp	2.07	0.30	-1.00	-0.01	-1.36	Trp	-0.57	0.51	0.55	-0.45	-0.05
Cys	1.36	0.70	-0.50	-0.71	-0.85	Cys	-0.87	0.32	0.25	0.27	0.03
Ser	1.48	0.67	-0.63	-0.97	-0.54	Ser	-0.75	0.59	0.29	0.04	-0.17
Thr	1.27	0.76	-0.50	-0.84	-0.69	Thr	-0.65	0.24	0.28	0.17	-0.04
Asn	1.35	0.55	-0.86	-0.23	-0.81	Asn	-0.47	0.58	-0.12	-0.04	0.05
Gln	1.14	1.45	-0.81	-1.26	-0.52	Gln	-0.96	0.65	0.48	0.07	-0.25
Asp	0.56	1.09	-0.72	-0.44	-0.50	Asp	-1.46	1.86	0.21	-0.91	0.29
Glu	0.92	0.87	0.28	-1.32	-0.74	Glu	-1.61	0.94	1.00	-0.43	0.09
Lys	1.45	1.03	-0.51	-0.92	-1.06	Lys	-0.37	1.85	-1.19	0.02	-0.32
Arg	1.32	0.95	-0.59	-0.16	-1.52	Arg	-0.07	1.00	-1.18	0.33	-0.08

[a] AMBER99 dispersion correction.

M05-2X/6-31G**//M05-2X/6-31G**						M05-2X-D[a]/6-31G**//M05-2X/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	0.55	-0.74	-0.13	-0.26	0.58	Pro	-2.95	-3.29	2.29	3.72	0.23
Gly	0.47	-0.79	0.42	-0.47	0.36	Gly	-1.76	-1.82	1.32	0.79	1.47
Ala	0.69	-1.20	0.47	-0.17	0.20	Ala	-1.59	-1.90	1.44	0.91	1.13
Val	0.60	-1.53	0.84	-0.06	0.15	Val	-1.75	-0.99	1.05	0.61	1.09
Leu	0.35	-1.39	0.85	-0.29	0.48	Leu	-1.73	-1.49	1.42	0.48	1.32
Ile	0.56	-1.64	0.85	0.08	0.14	Ile	-1.60	-0.49	1.13	0.95	0.01
Met	0.37	-1.53	0.60	-0.12	0.68	Met	-1.59	-1.83	1.42	0.80	1.19
Phe	0.71	-1.98	0.65	0.64	-0.03	Phe	-0.99	-1.49	0.39	0.53	1.56
Tyr	0.68	-1.93	0.71	0.60	-0.05	Tyr	-1.03	-1.49	0.34	0.47	1.71
His	0.60	-1.87	0.55	0.54	0.18	His	-0.97	-1.35	-0.04	0.65	1.72
Trp	0.97	-1.99	0.02	0.89	0.10	Trp	-1.67	-1.77	1.57	0.46	1.41
Cys	0.56	-1.83	0.72	0.09	0.46	Cys	-1.67	-2.21	1.47	1.06	1.35
Ser	0.59	-1.48	0.49	-0.13	0.53	Ser	-1.64	-1.56	1.41	0.88	0.91
Thr	0.48	-2.40	1.23	0.27	0.42	Thr	-1.45	-2.91	2.01	1.28	1.06
Asn	0.60	-1.75	-0.07	0.73	0.50	Asn	-1.22	-1.72	0.67	0.92	1.36
Gln	0.24	-1.01	0.36	-0.51	0.92	Gln	-1.86	-1.81	1.65	0.83	1.19
Asp	0.52	-0.64	-1.13	-0.15	1.39	Asp	-1.49	0.12	-0.20	-0.61	2.19
Glu	0.65	-0.97	-0.43	-0.04	0.79	Glu	-1.87	-0.89	0.29	0.85	1.63
Lys	0.38	-1.25	0.80	-0.16	0.23	Lys	-1.43	-0.44	0.11	0.78	0.98
Arg	0.84	-1.21	0.61	-0.40	0.17	Arg	-0.56	-1.16	0.02	0.09	1.61

PBE/cc-pVTZ//PBE/6-31G**						PBE-D[a]/cc-pVTZ//PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	3.68	3.54	-3.24	-2.63	-1.35	Pro	0.18	0.98	-0.82	1.34	-1.69
Gly	3.69	3.75	-3.51	-3.29	-0.64	Gly	1.46	2.71	-2.61	-2.03	0.47
Ala	3.77	3.79	-3.58	-3.50	-0.48	Ala	1.49	3.09	-2.61	-2.41	0.44
Val	3.52	3.48	-3.42	-2.77	-0.81	Val	1.17	4.01	-3.20	-2.10	0.12
Leu	3.66	3.44	-3.29	-2.97	-0.85	Leu	1.58	3.34	-2.73	-2.19	-0.01
Ile	3.36	3.64	-3.45	-2.86	-0.68	Ile	1.19	4.79	-3.17	-2.00	-0.81
Met	3.10	3.92	-3.59	-3.38	-0.04	Met	1.14	3.61	-2.77	-2.46	0.48
Phe	3.19	3.11	-2.40	-1.80	-2.10	Phe	1.48	3.61	-2.66	-1.92	-0.51
Tyr	2.78	2.82	-1.79	-1.46	-2.35	Tyr	1.07	3.26	-2.16	-1.59	-0.59
His	3.57	3.01	-2.32	-2.44	-1.82	His	2.00	3.53	-2.91	-2.33	-0.29
Trp	4.10	3.15	-3.58	-1.92	-1.74	Trp	1.46	3.36	-2.03	-2.35	-0.44
Cys	3.71	4.13	-4.86	-2.46	-0.52	Cys	1.48	3.75	-4.11	-1.48	0.37
Ser	3.52	3.86	-3.73	-3.10	-0.55	Ser	1.29	3.78	-2.81	-2.09	-0.17
Thr	3.75	3.50	-3.44	-3.02	-0.79	Thr	1.83	2.99	-2.67	-2.00	-0.15
Asn	3.17	3.90	-3.15	-2.75	-1.17	Asn	1.35	3.93	-2.41	-2.55	-0.32
Gln	2.83	4.01	-3.81	-3.36	0.32	Gln	0.74	3.21	-2.52	-2.03	0.60
Asp	2.05	1.84	-1.67	-0.54	-1.68	Asp	0.04	2.61	-0.75	-1.01	-0.89
Glu	3.33	2.79	-2.17	-2.96	-0.98	Glu	0.80	2.87	-1.44	-2.08	-0.15
Lys	3.89	3.16	-3.52	-2.83	-0.70	Lys	2.07	3.98	-4.20	-1.89	0.04
Arg	2.59	3.50	-3.49	-1.68	-0.94	Arg	1.20	3.56	-4.08	-1.19	0.51

[a] AMBER99 dispersion correction.

PBE/6-31G**//PBE/6-31G**						PBE-D[a]/6-31G**//PBE/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	2.52	1.37	-2.59	-1.86	0.57	Pro	-0.98	-1.19	-0.17	2.11	0.23
Gly	2.45	1.77	-2.25	-2.39	0.43	Gly	0.21	0.73	-1.35	-1.13	1.53
Ala	2.69	1.50	-2.25	-2.38	0.45	Ala	0.41	0.80	-1.29	-1.30	1.37
Val	2.50	1.01	-1.85	-1.68	0.02	Val	0.15	1.55	-1.64	-1.01	0.95
Leu	2.38	1.19	-1.76	-2.09	0.28	Leu	0.30	1.10	-1.20	-1.32	1.12
Ile	2.37	1.08	-1.87	-1.75	0.18	Ile	0.20	2.23	-1.59	-0.88	0.04
Met	2.02	1.50	-2.13	-2.27	0.87	Met	0.07	1.20	-1.31	-1.35	1.39
Phe	2.16	0.82	-1.36	-0.66	-0.95	Phe	0.46	1.31	-1.63	-0.77	0.63
Tyr	1.83	0.58	-0.92	-0.30	-1.18	Tyr	0.12	1.02	-1.30	-0.42	0.58
His	2.41	0.78	-1.22	-1.32	-0.65	His	0.83	1.31	-1.81	-1.21	0.88
Trp	2.85	0.83	-2.37	-0.70	-0.61	Trp	0.21	1.04	-0.82	-1.14	0.70
Cys	2.68	1.65	-3.45	-1.50	0.63	Cys	0.45	1.27	-2.71	-0.53	1.52
Ser	2.39	1.69	-2.39	-2.05	0.36	Ser	0.16	1.61	-1.48	-1.04	0.74
Thr	2.61	0.39	-1.55	-1.70	0.24	Thr	0.69	-0.13	-0.77	-0.68	0.89
Asn	2.22	1.51	-2.07	-1.60	-0.06	Asn	0.40	1.54	-1.33	-1.41	0.80
Gln	1.73	1.54	-2.43	-2.40	1.55	Gln	-0.37	0.74	-1.14	-1.06	1.82
Asp	1.50	0.51	-2.31	0.23	0.07	Asp	-0.52	1.28	-1.38	-0.24	0.86
Glu	2.77	1.24	-2.57	-1.62	0.18	Glu	0.25	1.32	-1.85	-0.73	1.02
Lys	2.56	0.90	-2.07	-1.83	0.45	Lys	0.74	1.71	-2.76	-0.89	1.19
Arg	2.06	1.30	-1.88	-2.14	0.66	Arg	0.67	1.36	-2.47	-1.66	2.10

[a] AMBER99 dispersion correction.

B3LYP/cc-pVTZ//B3LYP/6-31G**						B3LYP-D[a]/cc-pVTZ//B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	4.32	4.47	-3.32	-2.96	-2.52	Pro	0.83	1.91	-0.90	1.02	-2.86
Gly	4.37	4.57	-3.85	-3.37	-1.72	Gly	2.13	3.53	-2.94	-2.10	-0.61
Ala	4.50	4.83	-3.88	-4.05	-1.41	Ala	2.23	4.13	-2.91	-2.96	-0.48
Val	4.17	4.46	-3.79	-3.22	-1.62	Val	1.81	5.00	-3.58	-2.55	-0.69
Leu	4.41	4.42	-3.61	-3.39	-1.83	Leu	2.33	4.32	-3.05	-2.62	-0.98
Ile	4.04	4.73	-3.83	-3.28	-1.65	Ile	1.88	5.88	-3.55	-2.42	-1.79
Met	3.68	5.10	-4.04	-3.99	-0.74	Met	1.72	4.80	-3.22	-3.07	-0.23
Phe	3.84	4.02	-2.50	-2.19	-3.17	Phe	2.14	4.52	-2.77	-2.30	-1.59
Tyr	3.48	3.75	-2.02	-1.76	-3.45	Tyr	1.77	4.19	-2.39	-1.89	-1.68
His	4.25	3.81	-2.38	-2.79	-2.89	His	2.68	4.33	-2.97	-2.69	-1.36
Trp	4.98	4.02	-3.91	-2.30	-2.79	Trp	2.34	4.23	-2.36	-2.74	-1.48
Cys	4.50	4.98	-5.08	-2.87	-1.53	Cys	2.27	4.60	-4.33	-1.90	-0.64
Ser	4.38	4.67	-4.15	-3.67	-1.23	Ser	2.15	4.59	-3.23	-2.66	-0.85
Thr	4.48	4.62	-3.91	-3.49	-1.70	Thr	2.56	4.10	-3.14	-2.47	-1.05
Asn	3.91	4.75	-3.53	-2.99	-2.14	Asn	2.09	4.78	-2.79	-2.80	-1.28
Gln	3.44	5.17	-4.21	-3.94	-0.46	Gln	1.34	4.37	-2.92	-2.61	-0.19
Asp	2.11	2.84	-1.77	-0.90	-2.29	Asp	0.10	3.61	-0.84	-1.37	-1.50
Glu	3.60	3.30	-1.28	-3.62	-2.00	Glu	1.08	3.37	-0.55	-2.73	-1.17
Lys	4.65	4.23	-3.82	-3.29	-1.76	Lys	2.83	5.04	-4.50	-2.35	-1.02
Arg	3.08	4.52	-3.89	-1.40	-2.30	Arg	1.69	4.57	-4.49	-0.91	-0.86

[a] AMBER99 dispersion correction.

B3LYP/6-31G**//B3LYP/6-31G**						B3LYP-D[a]/6-31G**//B3LYP/6-31G**					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	3.12	2.34	-2.65	-2.19	-0.62	Pro	-0.38	-0.22	-0.23	1.79	-0.96
Gly	3.03	2.55	-2.63	-2.35	-0.59	Gly	0.79	1.51	-1.73	-1.09	0.52
Ala	3.36	2.51	-2.59	-2.94	-0.34	Ala	1.09	1.81	-1.62	-1.86	0.58
Val	3.07	2.03	-2.28	-2.15	-0.69	Val	0.72	2.57	-2.06	-1.48	0.25
Leu	3.05	2.18	-2.13	-2.52	-0.58	Leu	0.97	2.08	-1.57	-1.75	0.27
Ile	2.96	2.18	-2.31	-2.20	-0.63	Ile	0.79	3.33	-2.03	-1.33	-0.77
Met	2.57	2.68	-2.62	-2.90	0.27	Met	0.61	2.38	-1.80	-1.98	0.79
Phe	2.68	1.81	-1.48	-1.07	-1.94	Phe	0.98	2.30	-1.75	-1.18	-0.36
Tyr	2.31	1.49	-0.86	-0.69	-2.25	Tyr	0.60	1.93	-1.23	-0.82	-0.48
His	2.96	1.63	-1.27	-1.71	-1.61	His	1.39	2.15	-1.86	-1.60	-0.08
Trp	3.57	1.75	-2.62	-1.15	-1.55	Trp	0.93	1.96	-1.06	-1.59	-0.24
Cys	3.41	2.52	-3.69	-1.94	-0.29	Cys	1.18	2.14	-2.95	-0.96	0.59
Ser	3.22	2.50	-2.86	-2.63	-0.23	Ser	0.99	2.42	-1.94	-1.62	0.15
Thr	3.27	1.54	-2.05	-2.17	-0.58	Thr	1.35	1.02	-1.27	-1.16	0.06
Asn	2.92	2.31	-2.51	-1.85	-0.87	Asn	1.10	2.34	-1.77	-1.65	-0.01
Gln	2.30	2.68	-2.86	-2.98	0.86	Gln	0.20	1.89	-1.57	-1.65	1.13
Asp	1.61	1.54	-2.39	-0.35	-0.41	Asp	-0.41	2.31	-1.46	-0.82	0.38
Glu	2.82	1.70	-1.63	-2.28	-0.60	Glu	0.29	1.78	-0.90	-1.40	0.23
Lys	3.22	1.99	-2.41	-2.29	-0.52	Lys	1.41	2.81	-3.09	-1.34	0.22
Arg	2.45	2.36	-2.32	-1.83	-0.66	Arg	1.06	2.41	-2.91	-1.35	0.78

[a] AMBER99 dispersion correction.

AM1//AM1						AM1-D[a]//AM1					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	2.76	3.80	-3.88	-1.54	-1.14	Pro	-0.73	1.24	-1.46	2.44	-1.48
Gly	2.92	4.80	-4.02	-1.54	-2.16	Gly	0.68	3.76	-3.12	-0.27	-1.05
Ala	2.40	5.49	-3.84	-1.65	-2.40	Ala	0.12	4.79	-2.87	-0.57	-1.47
Val	1.81	5.16	-3.44	-0.78	-2.74	Val	-0.55	5.69	-3.22	-0.11	-1.81
Leu	3.03	4.29	-3.21	-1.37	-2.74	Leu	0.95	4.20	-2.65	-0.60	-1.90
Ile	1.82	5.36	-3.20	-0.72	-3.26	Ile	-0.35	6.51	-2.92	0.14	-3.39
Met	0.63	6.16	-3.95	-1.67	-1.17	Met	-1.33	5.86	-3.13	-0.75	-0.66
Phe	2.80	4.61	-2.88	-0.06	-4.47	Phe	1.10	5.10	-3.15	-0.17	-2.88
Tyr	2.45	4.20	-2.32	0.40	-4.73	Tyr	0.74	4.64	-2.69	0.28	-2.96
His	3.03	4.06	-2.69	-0.51	-3.89	His	1.46	4.58	-3.28	-0.40	-2.36
Trp	3.63	4.23	-3.47	-0.26	-4.12	Trp	0.99	4.44	-1.92	-0.69	-2.82
Cys	2.20	5.13	-4.13	-0.95	-2.26	Cys	-0.03	4.75	-3.38	0.03	-1.37
Ser	1.01	5.79	-4.15	0.75	-3.40	Ser	-1.22	5.72	-3.23	1.76	-3.02
Thr	1.46	4.94	-3.53	-1.16	-1.72	Thr	-0.46	4.43	-2.75	-0.14	-1.08
Asn	0.74	6.90	-2.24	-2.00	-3.41	Asn	-1.08	6.93	-1.49	-1.80	-2.56
Gln	0.48	5.38	-4.13	-1.70	-0.04	Gln	-1.61	4.58	-2.84	-0.36	0.23
Asp	0.60	5.37	-0.48	-1.66	-3.83	Asp	-1.42	6.14	0.44	-2.13	-3.04
Glu	3.03	3.37	0.07	-2.81	-3.67	Glu	0.51	3.45	0.80	-1.92	-2.83
Lys	2.54	4.72	-3.62	-1.14	-2.51	Lys	0.72	5.54	-4.30	-0.20	-1.76
Arg	-0.86	3.94	-4.96	5.28	-3.40	Arg	-2.25	4.00	-5.56	5.76	-1.96

[a] AMBER99 dispersion correction.

PM3//PM3						PM3-D[a]//PM3					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	6.69	8.45	-5.12	-5.14	-4.89	Pro	3.20	5.90	-2.70	-1.16	-5.23
Gly	5.72	7.37	-3.20	-2.42	-7.48	Gly	3.49	6.33	-2.29	-1.15	-6.37
Ala	6.10	8.61	-4.58	-2.86	-7.27	Ala	3.82	7.91	-3.61	-1.78	-6.34
Val	5.98	8.26	-4.63	-2.33	-7.27	Val	3.62	8.79	-4.41	-1.66	-6.34
Leu	7.39	7.14	-4.33	-2.43	-7.77	Leu	5.31	7.04	-3.77	-1.66	-6.93
Ile	5.82	8.60	-4.42	-2.47	-7.54	Ile	3.66	9.75	-4.14	-1.60	-7.67
Met	4.33	9.82	-4.95	-3.29	-5.91	Met	2.37	9.52	-4.13	-2.37	-5.40
Phe	5.81	7.91	-2.86	-1.43	-9.42	Phe	4.10	8.40	-3.13	-1.54	-7.84
Tyr	5.58	7.66	-2.85	-0.85	-9.54	Tyr	3.87	8.11	-3.23	-0.98	-7.77
His	6.12	8.41	-3.67	-2.12	-8.73	His	4.54	8.93	-4.27	-2.01	-7.20
Trp	6.80	7.86	-4.01	-1.66	-8.99	Trp	4.16	8.07	-2.46	-2.09	-7.68
Cys	5.65	8.24	-5.27	-1.66	-6.95	Cys	3.42	7.86	-4.53	-0.68	-6.06
Ser	4.17	8.12	-2.39	-3.05	-6.85	Ser	1.94	8.04	-1.47	-2.04	-6.47
Thr	7.37	8.33	-5.13	-3.72	-6.85	Thr	5.45	7.82	-4.35	-2.70	-6.21
Asn	3.96	9.97	-2.77	-2.97	-8.19	Asn	2.14	10.00	-2.02	-2.77	-7.33
Gln	4.10	8.54	-5.10	-3.00	-4.54	Gln	2.00	7.74	-3.81	-1.66	-4.27
Asp	5.01	8.90	-0.34	-5.95	-7.62	Asp	3.00	9.66	0.59	-6.42	-6.83
Glu	6.43	5.65	-0.46	-3.98	-7.64	Glu	3.91	5.73	0.26	-3.09	-6.81
Lys	5.99	8.62	-4.88	-2.47	-7.26	Lys	4.17	9.44	-5.57	-1.53	-6.52
Arg	2.40	8.27	-6.30	2.95	-7.32	Arg	1.01	8.32	-6.89	3.44	-5.87

[a] AMBER99 dispersion correction.

PM3MM//PM3MM						PM3MM-D[a]//PM3MM					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	6.65	8.95	-5.69	-5.46	-4.45	Pro	3.15	6.39	-3.27	-1.48	-4.79
Gly	6.42	8.50	-5.43	-3.17	-6.33	Gly	4.19	7.46	-4.53	-1.90	-5.22
Ala	6.18	9.38	-5.44	-3.59	-6.52	Ala	3.90	8.68	-4.47	-2.50	-5.60
Val	5.89	8.92	-5.35	-2.83	-6.63	Val	3.54	9.45	-5.13	-2.16	-5.70
Leu	7.30	7.91	-5.17	-2.96	-7.07	Leu	5.22	7.81	-4.61	-2.19	-6.23
Ile	5.79	9.20	-5.19	-2.98	-6.81	Ile	3.62	10.35	-4.91	-2.11	-6.94
Met	4.44	10.29	-5.77	-3.89	-5.07	Met	2.49	9.99	-4.95	-2.97	-4.56
Phe	5.99	8.85	-4.36	-1.78	-8.70	Phe	4.29	9.35	-4.63	-1.89	-7.12
Tyr	5.61	8.44	-3.77	-1.30	-8.98	Tyr	3.90	8.88	-4.15	-1.42	-7.22
His	6.06	8.90	-4.27	-2.42	-8.27	His	4.49	9.42	-4.86	-2.31	-6.74
Trp	6.78	8.59	-4.96	-1.91	-8.49	Trp	4.14	8.80	-3.41	-2.35	-7.18
Cys	6.16	9.24	-5.96	-3.33	-6.11	Cys	3.93	8.86	-5.21	-2.36	-5.23
Ser	4.94	9.90	-6.11	-1.36	-7.37	Ser	2.71	9.82	-5.19	-0.35	-6.99
Thr	7.87	9.79	-5.91	-6.31	-5.44	Thr	5.95	9.27	-5.13	-5.30	-4.80
Asn	4.69	10.91	-4.45	-3.61	-7.54	Asn	2.87	10.94	-3.71	-3.42	-6.68
Gln	4.38	9.52	-5.93	-3.98	-3.99	Gln	2.28	8.72	-4.64	-2.65	-3.72
Asp	5.07	6.23	0.87	-4.52	-7.66	Asp	3.06	7.00	1.79	-4.98	-6.87
Glu	5.41	7.22	-1.06	-4.34	-7.23	Glu	2.89	7.30	-0.34	-3.45	-6.40
Lys	6.86	9.39	-6.05	-3.47	-6.74	Lys	5.05	10.20	-6.73	-2.52	-6.00
Arg	3.66	8.98	-7.50	1.85	-7.00	Arg	2.27	9.03	-8.09	2.34	-5.56

[a] AMBER99 dispersion correction.

AMOEBA//AMOEBA						AMBEREP//AMBEREP					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-2.40	-3.07	2.75	6.01	-3.29	Pro	-12.74	36.30	-6.34	-6.53	-10.68
Gly	0.45	-0.05	0.27	0.66	-1.33	Gly	-0.87	5.01	-1.95	-2.82	0.62
Ala	0.78	-0.22	0.34	0.20	-1.10	Ala	-2.37	6.81	-1.22	-2.34	-0.89
Val	0.18	-0.61	1.01	1.79	-2.37	Val	-1.76	6.07	-1.30	-1.96	-1.05
Leu	0.31	-0.32	0.07	1.14	-1.20	Leu	-2.47	6.66	-0.73	-2.52	-0.94
Ile	-0.14	-1.01	0.71	1.55	-1.10	Ile	-2.45	8.04	-1.38	-2.30	-1.91
Met	-0.22	0.32	0.46	0.01	-0.56	Met	-3.24	6.71	-1.18	-2.41	0.11
Phe	-0.40	-0.75	0.65	1.42	-0.92	Phe	-3.00	7.02	-1.02	-1.29	-1.71
Tyr	-0.41	-1.09	0.89	1.60	-0.99	Tyr	-2.92	6.54	-0.87	-1.28	-1.47
His	2.68	-0.28	-0.14	-0.26	-2.01	His	-0.54	4.89	-1.65	-1.11	-1.59
Trp	0.61	-0.96	0.94	1.46	-2.05	Trp	-3.97	7.58	-0.49	-1.25	-1.87
Cys	1.80	0.00	-1.71	0.94	-1.03	Cys	-3.22	7.39	-0.37	-1.38	-2.42
Ser	0.02	-1.61	0.71	0.40	0.48	Ser	-2.42	6.36	-1.13	-2.29	-0.52
Thr	2.14	1.79	-0.47	0.15	-3.61	Thr	-2.31	7.36	-0.63	-1.20	-3.23
Asn	2.08	1.04	-0.14	-2.64	-0.34	Asn	-2.73	8.98	-0.58	-4.61	-1.05
Gln	0.19	1.52	-0.79	-0.64	-0.27	Gln	-2.40	6.50	-0.87	-1.73	-1.50
Asp	0.11	-3.93	4.95	0.08	-1.21	Asp	-1.74	2.35	1.11	-2.48	0.75
Glu	-0.57	-1.62	3.03	1.44	-2.28	Glu	-5.89	7.82	1.53	-3.08	-0.37
Lys	2.32	-1.01	-0.52	0.91	-1.70	Lys	-1.70	7.38	-1.97	-2.29	-1.41
Arg	-0.48	0.51	0.59	0.73	-1.35	Arg	-3.04	6.34	-2.57	1.19	-1.93

AMBERPOL//AMBERPOL						AMBER94//AMBER94					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-4.65	1.18	3.33	3.58	-3.43	Pro	-5.22	0.92	1.60	4.96	-2.27
Gly	-1.12	4.52	-0.71	-0.57	-2.12	Gly	-2.69	3.63	-0.05	0.68	-1.56
Ala	-2.58	6.27	-0.17	-0.85	-2.67	Ala	-4.16	5.95	0.32	0.31	-2.42
Val	-1.84	5.25	-0.41	-0.52	-2.47	Val	-3.55	5.13	0.02	0.43	-2.04
Leu	-2.63	6.05	0.22	-1.19	-2.45	Leu	-4.38	5.66	-0.56	1.02	-1.75
Ile	-2.70	7.34	-0.35	-0.80	-3.49	Ile	-3.17	5.72	0.30	0.75	-3.60
Met	-3.62	6.85	-0.42	-1.14	-1.67	Met	-4.56	5.09	0.41	0.08	-1.02
Phe	-3.07	6.34	-0.18	0.01	-3.10	Phe	-4.74	6.06	0.27	1.19	-2.78
Tyr	-3.22	6.31	-0.01	0.27	-3.34	Tyr	-4.58	5.38	0.54	1.57	-2.90
His	-1.37	5.25	-0.71	-0.20	-2.98	His	-4.40	4.99	0.39	1.66	-2.64
Trp	-4.01	6.63	0.58	0.09	-3.29	Trp	-4.67	5.28	0.98	1.23	-2.82
Cys	-2.43	6.59	-0.37	-0.78	-3.00	Cys	-4.03	4.54	0.99	1.12	-2.63
Ser	-2.23	5.63	-0.35	-1.06	-1.99	Ser	-3.42	3.09	1.38	1.39	-2.44
Thr	-3.51	8.52	-0.67	-0.71	-3.64	Thr	-4.31	5.86	-0.56	0.07	-1.05
Asn	-1.87	7.83	-0.19	-3.46	-2.31	Asn	-2.74	4.73	-1.03	0.75	-1.71
Gln	-2.43	5.94	-0.06	-0.42	-3.04	Gln	-4.94	6.89	0.39	0.45	-2.79
Asp	-1.14	1.50	1.81	-1.42	-0.76	Asp	-4.84	2.05	2.41	0.27	0.10
Glu	-5.62	6.97	2.33	-1.58	-2.09	Glu	-7.24	5.71	3.59	-0.94	-1.11
Lys	-2.01	6.83	-1.59	-0.69	-2.54	Lys	-3.66	5.28	0.20	1.32	-3.14
Arg	-3.74	6.39	-1.83	2.23	-3.05	Arg	-5.22	5.10	-0.58	4.77	-4.08

AMBER96//AMBER96						AMBER99//AMBER99					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-0.35	5.79	-2.09	-0.15	-3.20	Pro	-3.54	0.57	2.08	1.76	-0.88
Gly	2.17	8.50	-3.75	-4.43	-2.49	Gly	-1.31	3.01	0.90	-2.34	-0.25
Ala	0.71	10.82	-3.38	-4.80	-3.35	Ala	-2.31	4.82	1.00	-2.66	-0.85
Val	1.32	10.00	-3.67	-4.68	-2.97	Val	-1.68	3.98	0.70	-2.53	-0.46
Leu	0.49	10.53	-4.25	-4.09	-2.68	Leu	-2.55	4.52	0.09	-1.89	-0.18
Ile	1.69	10.58	-3.40	-4.36	-4.53	Ile	-1.25	4.45	0.99	-2.20	-1.99
Met	0.30	9.96	-3.28	-5.03	-1.95	Met	-2.70	3.95	1.09	-2.90	0.56
Phe	0.13	10.93	-3.43	-3.92	-3.71	Phe	-2.88	4.94	0.94	-1.79	-1.21
Tyr	0.28	10.24	-3.15	-3.54	-3.83	Tyr	-2.73	4.25	1.21	-1.40	-1.33
His	0.47	9.85	-3.30	-3.45	-3.57	His	-2.55	3.86	1.06	-1.30	-1.07
Trp	0.19	10.14	-2.71	-3.88	-3.75	Trp	-2.82	4.17	1.64	-1.75	-1.25
Cys	0.84	9.41	-2.70	-3.99	-3.56	Cys	-2.18	3.40	1.67	-1.84	-1.06
Ser	1.45	7.96	-2.31	-3.72	-3.37	Ser	-1.58	1.93	2.07	-1.57	-0.85
Thr	0.55	10.72	-4.26	-5.04	-1.98	Thr	-2.43	4.63	0.14	-2.89	0.55
Asn	2.13	9.60	-4.73	-4.36	-2.64	Asn	-1.03	3.43	-0.52	-1.61	-0.27
Gln	-0.07	11.76	-3.31	-4.66	-3.71	Gln	-3.36	6.18	0.80	-2.79	-0.83
Asp	0.03	6.92	-1.28	-4.84	-0.83	Asp	-2.99	0.76	3.28	-2.71	1.65
Glu	-2.37	10.57	-0.11	-6.05	-2.04	Glu	-5.46	4.87	4.18	-3.99	0.40
Lys	1.21	10.14	-3.49	-3.79	-4.06	Lys	-1.80	4.19	0.86	-1.67	-1.58
Arg	-0.35	9.97	-4.27	-0.34	-5.01	Arg	-3.41	4.02	0.03	1.94	-2.58

AMBER99SB//AMBER99SB						AMBER03//AMBER03					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	1.50	2.00	1.01	0.10	-4.60	Pro	-1.22	6.40	1.58	-1.36	-5.40
Gly	2.94	3.03	-0.48	-1.82	-3.67	Gly	0.49	7.38	-1.68	-2.22	-3.97
Ala	3.00	3.83	-0.53	-2.59	-3.71	Ala	-0.41	10.89	-1.88	-3.65	-4.96
Val	3.64	3.00	-0.81	-2.47	-3.35	Val	1.23	8.32	-2.30	-3.75	-3.50
Leu	2.75	3.56	-1.44	-1.84	-3.03	Leu	-0.61	10.67	-2.44	-2.74	-4.88
Ile	4.10	3.50	-0.50	-2.10	-5.00	Ile	1.61	12.44	-3.15	-4.50	-6.39
Met	2.59	2.96	-0.45	-2.83	-2.27	Met	-1.07	8.75	-0.95	-3.02	-3.71
Phe	2.40	3.95	-0.59	-1.72	-4.05	Phe	-1.29	9.15	-1.13	-1.84	-4.89
Tyr	2.56	3.25	-0.31	-1.30	-4.19	Tyr	-3.81	8.59	0.12	-0.47	-4.43
His	2.79	2.88	-0.45	-1.21	-4.00	His	-3.75	7.64	0.36	-0.10	-4.15
Trp	2.48	3.19	0.10	-1.64	-4.12	Trp	-2.86	7.84	-0.59	-0.80	-3.59
Cys	3.14	2.45	-0.01	-1.75	-3.82	Cys	-0.42	8.96	-0.98	-2.45	-5.11
Ser	3.74	0.98	0.52	-1.54	-3.71	Ser	-0.25	9.85	-1.42	-3.35	-4.85
Thr	3.53	3.41	-1.34	-2.78	-2.83	Thr	1.19	11.90	-2.97	-3.20	-6.92
Asn	4.11	2.49	-2.11	-1.33	-3.17	Asn	0.12	7.21	-2.46	-1.40	-3.46
Gln	1.64	5.76	-1.01	-3.03	-3.36	Gln	0.15	15.16	-3.68	-5.75	-5.88
Asp	2.26	-0.26	1.81	-2.60	-1.21	Asp	-2.39	7.13	1.05	-4.24	-1.54
Glu	-0.11	3.74	2.72	-3.88	-2.47	Glu	-0.95	11.31	0.94	-6.64	-4.66
Lys	3.50	3.25	-0.66	-1.62	-4.46	Lys	4.20	6.53	-2.10	-1.96	-6.67
Arg	1.88	3.05	-1.50	2.05	-5.49	Arg	-0.87	5.85	-2.41	4.50	-7.06

CHARMM27//CHARMM27						OPLS-AA//OPLS-AA					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-1.62	9.44	-1.12	-0.22	-6.49	Pro	-0.28	0.53	-1.45	6.28	-5.07
Gly	0.35	12.07	-4.99	-3.66	-3.78	Gly	2.47	4.60	-2.85	-2.36	-1.87
Ala	-2.18	15.85	-4.35	-3.33	-5.99	Ala	2.36	5.94	-3.16	-2.65	-2.48
Val	-2.31	16.01	-4.80	-2.77	-6.13	Val	2.45	5.64	-3.10	-2.04	-2.96
Leu	-1.68	15.07	-4.73	-2.43	-6.23	Leu	2.90	5.24	-3.43	-2.05	-2.66
Ile	-2.16	16.48	-4.64	-2.62	-7.06	Ile	2.83	6.44	-2.79	-1.69	-4.78
Met	-2.64	16.17	-4.55	-3.80	-5.18	Met	1.22	6.83	-4.29	-4.09	0.32
Phe	-1.24	15.00	-4.33	-2.29	-7.13	Phe	3.42	4.23	-2.94	-1.14	-3.57
Tyr	-1.36	14.65	-4.03	-1.97	-7.29	Tyr	3.27	3.87	-2.60	-0.80	-3.74
His	0.05	11.89	-3.53	-1.66	-6.75	His	3.14	3.83	-2.59	-1.19	-3.20
Trp	-1.57	14.58	-4.41	-2.18	-6.43	Trp	1.44	5.84	-4.40	-0.41	-2.47
Cys	-1.64	15.12	-4.29	-2.66	-6.53	Cys	3.41	4.75	-3.71	-2.32	-2.13
Ser	-1.89	13.15	-4.35	-3.33	-3.58	Ser	3.11	4.14	-3.23	-2.63	-1.40
Thr	-2.28	16.74	-5.56	-3.39	-5.51	Thr	3.37	4.57	-2.66	-1.38	-3.89
Asn	-1.91	15.70	-2.81	-4.36	-6.63	Asn	4.58	3.16	-5.95	-0.87	-0.92
Gln	-3.04	17.05	-4.72	-3.59	-5.70	Gln	1.94	5.06	-1.63	-1.17	-4.20
Asp	-7.56	14.07	2.83	-3.02	-6.32	Asp	0.92	-0.76	-2.87	2.55	0.17
Glu	-6.42	15.56	-0.12	-3.13	-5.89	Glu	-0.31	4.63	1.89	-3.21	-3.00
Lys	-0.82	14.95	-4.97	-2.67	-6.48	Lys	4.43	5.62	-4.16	-2.57	-3.31
Arg	-2.26	14.82	-5.82	1.29	-8.03	Arg	1.41	5.66	-4.72	2.55	-4.89

OPLS-AA/L//OPLS-AA/L						AMBERUA//AMBERUA					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-0.57	1.17	-0.62	6.72	-6.70	Pro	-9.93	43.01	-9.24	-8.63	-15.21
Gly	4.79	7.77	-5.54	-5.07	-1.95	Gly	0.21	9.34	-2.27	-3.00	-4.28
Ala	1.92	6.81	-2.01	-2.98	-3.75	Ala	-2.34	12.04	-1.52	-3.33	-4.84
Val	1.92	6.39	-2.00	-2.45	-3.86	Val	-0.17	8.37	-0.84	-2.09	-5.26
Leu	2.65	5.88	-2.03	-2.35	-4.15	Leu	-2.73	11.77	-1.73	-2.73	-4.58
Ile	1.65	6.75	-2.32	-2.71	-3.36	Ile	-1.71	10.14	-0.99	-2.33	-5.11
Met	0.81	7.77	-3.24	-4.42	-0.92	Met	-2.35	10.15	-1.24	-2.94	-3.62
Phe	2.96	5.06	-1.83	-1.26	-4.94	Phe	-2.59	11.38	-1.17	-2.09	-5.53
Tyr	2.81	4.68	-1.53	-0.88	-5.09	Tyr	-5.73	10.77	0.19	-0.61	-4.62
His	2.91	4.03	-1.48	-1.18	-4.28	His	-3.01	10.54	-0.71	-1.59	-5.23
Trp	1.42	6.19	-2.90	-0.80	-3.91	Trp	-3.54	10.50	-0.52	-1.43	-5.00
Cys	3.48	6.25	-3.34	-3.51	-2.88	Cys	-2.38	10.79	-1.01	-2.37	-5.03
Ser	3.44	5.88	-1.28	-2.49	-5.55	Ser	-2.98	9.06	-1.11	-2.75	-2.23
Thr	2.62	5.68	-1.75	-1.73	-4.82	Thr	-1.91	13.84	-3.50	-4.65	-3.78
Asn	3.38	6.02	-2.29	-3.85	-3.26	Asn	-0.40	10.08	-3.03	-2.24	-4.40
Gln	1.90	6.60	-1.92	-2.40	-4.19	Gln	-1.89	13.20	-1.63	-3.48	-6.19
Asp	-2.12	1.94	1.61	0.91	-2.35	Asp	-3.02	9.11	-0.08	-2.93	-3.08
Glu	-3.06	7.12	0.86	-2.06	-2.86	Glu	-2.75	10.54	1.52	-4.86	-4.45
Lys	3.35	6.52	-2.90	-2.63	-4.33	Lys	-1.86	9.53	-1.22	-1.78	-4.67
Arg	1.33	6.22	-3.54	2.12	-6.14	Arg	-1.92	7.65	-2.57	3.27	-6.43

GROMOS(G43b1)//GROMOS(G43b1)						GROMOS(G45a3)// GROMOS(G45a3)					
	α_R	α_L	β	β_a	PPII		α_R	α_L	β	β_a	PPII
Pro	-6.29	36.22	-10.33	-7.15	-12.45	Pro	-5.27	35.03	-10.40	-7.31	-12.05
Gly	3.97	6.62	-5.46	-2.77	-2.36	Gly	4.50	5.46	-5.36	-2.66	-1.95
Ala	3.59	7.81	-5.59	-3.19	-2.61	Ala	4.33	6.01	-5.42	-3.00	-1.92
Val	3.71	6.53	-5.07	-1.91	-3.26	Val	4.02	5.95	-5.18	-1.86	-2.93
Leu	4.04	6.74	-5.37	-2.88	-2.53	Leu	4.64	4.93	-5.52	-2.28	-1.77
Ile	3.47	7.17	-5.20	-2.08	-3.36	Ile	3.70	6.04	-5.31	-1.91	-2.53
Met	2.62	8.87	-5.88	-3.42	-2.19	Met	3.07	7.67	-5.88	-3.31	-1.56
Phe	2.84	8.42	-5.39	-2.74	-3.12	Phe	3.57	7.03	-5.37	-2.60	-2.63
Tyr	2.66	8.11	-4.97	-2.89	-2.91	Tyr	3.26	6.70	-5.01	-2.52	-2.43
His	2.93	7.97	-4.57	-2.41	-3.92	His	3.45	6.42	-4.63	-1.67	-3.57
Trp	1.57	8.41	-4.06	-2.36	-3.57	Trp	2.24	7.00	-3.88	-2.16	-3.20
Cys	3.79	8.70	-5.83	-2.90	-3.76	Cys	4.39	7.31	-5.76	-2.72	-3.22
Ser	2.67	7.56	-5.36	-2.82	-2.05	Ser	3.25	6.14	-5.28	-2.65	-1.46
Thr	3.99	6.16	-4.96	-2.59	-2.59	Thr	4.26	5.56	-5.23	-2.60	-1.98
Asn	3.59	8.88	-4.53	-4.56	-3.39	Asn	4.17	7.51	-4.39	-4.42	-2.88
Gln	2.61	8.13	-5.02	-2.36	-3.36	Gln	2.99	6.97	-5.20	-2.34	-2.41
Asp	12.00	-5.13	4.12	-2.23	-8.76	Asp	3.64	4.46	4.41	-4.90	-7.62
Glu	3.04	4.17	5.74	-5.11	-7.84	Glu	1.21	4.37	6.98	-5.50	-7.06
Lys	4.23	6.34	-6.76	-2.73	-1.08	Lys	4.43	3.93	-6.28	-1.60	-0.49
Arg	-4.46	6.74	-8.06	8.50	-2.73	Arg	0.06	3.02	-7.67	7.13	-2.54

GROMOS(G53a6)// GROMOS(G53a6)					
	α_R	α_L	β	β_a	PPII
Pro	-7.93	34.56	-12.85	2.57	-16.35
Gly	6.14	7.00	-6.57	-4.34	-2.24
Ala	5.95	7.63	-6.63	-4.67	-2.29
Val	5.49	7.71	-6.58	-3.47	-3.15
Leu	6.59	6.62	-6.59	-3.59	-3.03
Ile	5.25	7.93	-6.62	-3.42	-3.15
Met	4.32	6.75	-6.07	-4.01	-0.98
Phe	5.44	7.99	-6.46	-3.76	-3.21
Tyr	5.11	7.71	-6.11	-3.72	-3.00
His	4.89	7.58	-6.58	-2.70	-3.19
Trp	4.15	8.13	-5.11	-3.14	-4.04
Cys	6.16	7.07	-6.39	-4.16	-2.67
Ser	5.16	6.97	-5.65	-3.66	-2.83
Thr	5.54	7.83	-5.86	-3.23	-4.28
Asn	5.26	8.58	-6.23	-4.04	-3.57
Gln	4.23	9.96	-6.23	-3.90	-4.06
Asp	3.25	7.41	1.71	-5.80	-6.56
Glu	2.96	5.61	3.59	-6.41	-5.74
Lys	5.82	5.93	-7.03	-3.09	-1.63
Arg	2.62	4.98	-8.54	4.57	-3.62

Table S2c. Signed RMS-C (kcal/mol) of each conformation over 20 amino acids for each method.

	α_R	α_L	β	β_a	PPII	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.38	0.91	-0.58	-0.85	-1.02	0.95	0.26
M05-2X-D[a]/cc-pVTZ	-0.90	1.04	0.67	0.75	-0.46	0.76	0.20
M05-2X/6-31G**	0.59	-1.53	0.67	0.41	0.53	0.75	0.40
M05-2X-D[a]/6-31G**	-1.61	-1.71	1.22	1.13	1.34	1.40	0.22
PBE/cc-pVTZ	3.40	3.46	-3.29	-2.69	-1.19	2.80	0.85
PBE-D[a]/cc-pVTZ	1.35	3.43	-2.78	-2.00	-0.58	2.03	1.01
PBE/6-31G**	2.36	1.23	-2.14	-1.75	0.65	1.62	0.62
PBE-D[a]/6-31G**	0.48	1.29	-1.62	-1.13	1.13	1.13	0.37
B3LYP/cc-pVTZ	4.06	4.40	-3.56	-3.09	-2.09	3.44	0.81
B3LYP-D[a]/cc-pVTZ	2.00	4.36	-3.06	-2.38	-1.27	2.62	1.05
B3LYP/6-31G**	2.93	2.15	-2.39	-2.13	-0.98	2.12	0.64
B3LYP-D[a]/6-31G**	0.93	2.16	-1.86	-1.46	0.54	1.39	0.59
AM1	2.23	4.96	-3.42	-1.78	-3.09	3.09	1.10
AM1-D[a]	-1.05	4.97	-2.98	1.67	-2.21	2.58	1.35
PM3	5.70	8.28	-4.15	-3.07	-7.51	5.74	1.96
PM3-D[a]	3.63	8.26	-3.72	-2.44	-6.62	4.93	2.16
PM3MM	5.90	9.01	-5.20	-3.49	-6.95	6.11	1.83
PM3MM-D[a]	3.83	8.96	-4.75	-2.76	-6.06	5.27	2.14
AMOEBA	1.28	-1.46	1.58	1.76	-1.71	1.56	0.18
AMBEREP	-3.95	10.46	-1.91	-2.63	-2.81	4.35	3.12
AMBERPOL	-3.01	6.17	1.19	-1.45	-2.76	2.92	1.77
AMBER94	-4.44	5.05	1.19	1.80	-2.43	2.98	1.50
AMBER96	1.13	9.82	-3.31	-4.19	-3.30	4.35	2.91
AMBER99	-2.71	4.02	1.61	-2.27	-1.16	2.36	0.99
AMBER99SB	2.89	3.22	-1.15	-2.16	-3.75	2.63	0.90
AMBER03	-1.91	9.39	-1.95	-3.35	-4.98	4.31	2.77
CHARMM27	-2.84	14.83	-4.27	-2.88	-6.24	6.21	4.48
OPLS-AA	2.74	4.83	-3.39	-2.55	-3.17	3.34	0.81
OPLS-AA/L	2.65	5.97	-2.49	-3.01	-4.19	3.66	1.30
AMBERUA	-3.37	14.09	-2.63	-3.38	-5.74	5.84	4.26
GROMOS(G43b1)	4.43	10.84	-5.78	-3.77	-4.70	5.90	2.55
GROMOS(G45a3)	3.72	9.81	-5.82	-3.65	-4.21	5.44	2.32
GROMOS(G53a6)	5.26	10.58	-6.67	-4.02	-5.04	6.31	2.30

[1] Standard deviation. [a] AMBER99 dispersion correction.

Table S2d. RMS (kcal/mol) over the five conformations of each tetrapeptide for each method.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.19	1.11	1.10	1.00	0.96	0.98	0.91	0.95	0.93	0.89	1.20	0.87	0.92	0.85	0.85	1.09	0.70	0.89	1.04	1.03	0.97	0.12
M05-2X-D[a]/cc-pVTZ	2.04	0.37	0.39	0.87	0.53	1.14	0.43	0.40	0.40	0.47	0.47	0.45	0.45	0.35	0.34	0.57	1.14	0.97	1.01	0.71	0.67	0.41
M05-2X/6-31G**	0.50	0.52	0.66	0.83	0.79	0.87	0.81	1.03	1.01	0.95	1.07	0.94	0.78	1.24	0.92	0.68	0.89	0.66	0.70	0.74	0.83	0.18
M05-2X-D[a]/6-31G**	2.78	1.48	1.44	1.16	1.35	1.00	1.41	1.10	1.15	1.11	1.46	1.60	1.32	1.87	1.23	1.52	1.22	1.25	0.87	0.92	1.36	0.40
PBE/cc-pVTZ	3.01	3.20	3.28	2.98	3.02	3.00	3.14	2.58	2.31	2.70	3.04	3.49	3.20	3.10	2.97	3.16	1.64	2.58	3.03	2.64	2.90	0.40
PBE-D[a]/cc-pVTZ	1.12	2.03	2.22	2.53	2.28	2.80	2.38	2.29	1.97	2.47	2.16	2.66	2.38	2.16	2.44	2.08	1.35	1.75	2.87	2.55	2.22	0.43
PBE/6-31G**	1.94	2.00	2.02	1.65	1.71	1.64	1.83	1.31	1.10	1.42	1.75	2.21	1.93	1.57	1.68	1.97	1.26	1.92	1.74	1.70	1.72	0.28
PBE-D[a]/6-31G**	1.18	1.10	1.10	1.19	1.07	1.29	1.18	1.06	0.81	1.26	0.85	1.53	1.13	0.68	1.18	1.14	0.96	1.16	1.63	1.76	1.16	0.25
B3LYP/cc-pVTZ	3.60	3.71	3.93	3.60	3.66	3.66	3.80	3.23	3.01	3.30	3.73	4.03	3.83	3.79	3.57	3.80	2.08	2.92	3.69	3.23	3.51	0.44
B3LYP-D[a]/cc-pVTZ	1.70	2.47	2.81	3.10	2.87	3.46	3.03	2.84	2.56	2.96	2.78	3.13	2.96	2.84	2.98	2.69	1.89	2.08	3.47	3.01	2.78	0.45
B3LYP/6-31G**	2.34	2.39	2.57	2.18	2.25	2.20	2.41	1.87	1.66	1.93	2.30	2.66	2.52	2.11	2.21	2.46	1.48	1.95	2.27	2.04	2.19	0.29
B3LYP-D[a]/6-31G**	0.93	1.21	1.47	1.65	1.47	1.91	1.66	1.47	1.14	1.59	1.30	1.79	1.63	1.08	1.58	1.42	1.30	1.10	2.06	1.89	1.48	0.30
AM1	2.86	3.31	3.44	3.16	3.08	3.27	3.41	3.39	3.21	3.11	3.47	3.29	3.58	2.94	3.71	3.13	3.06	2.89	3.14	4.01	3.27	0.27
AM1-D[a]	1.57	2.26	2.60	3.05	2.43	3.54	3.06	3.02	2.76	2.82	2.56	2.68	3.37	2.39	3.50	2.52	3.27	2.21	3.25	4.22	2.85	0.57
PM3	6.21	5.64	6.22	6.06	6.17	6.17	6.09	6.25	6.16	6.36	6.45	5.98	5.39	6.49	6.30	5.39	6.29	5.44	6.21	5.93	6.06	0.33
PM3-D[a]	4.03	4.46	5.17	5.53	5.34	6.11	5.44	5.67	5.52	5.91	5.51	5.12	4.83	5.58	5.83	4.46	6.17	4.56	6.04	5.73	5.35	0.59
PM3MM	6.42	6.21	6.50	6.24	6.35	6.33	6.32	6.52	6.31	6.46	6.63	6.44	6.57	7.24	6.79	5.94	5.37	5.54	6.77	6.37	6.37	0.40
PM3MM-D[a]	4.16	4.99	5.44	5.75	5.53	6.28	5.66	6.03	5.75	6.06	5.71	5.55	6.00	6.31	6.29	4.97	5.17	4.79	6.59	6.14	5.66	0.59
AMOEBA	3.73	0.71	0.64	1.43	0.77	1.01	0.37	0.89	1.07	1.51	1.30	1.27	0.83	2.05	1.58	0.83	2.88	1.97	1.44	0.80	1.35	0.79
AMBEREP	18.32	2.76	3.46	3.05	3.41	4.04	3.54	3.58	3.34	2.48	3.96	3.82	3.26	3.79	4.71	3.29	1.81	4.64	3.70	3.50	4.22	3.30
AMBERPOL	3.43	2.32	3.28	2.74	3.20	3.85	3.59	3.44	3.51	2.79	3.77	3.44	2.89	4.45	4.06	3.18	1.37	4.30	3.47	3.81	3.34	0.68
AMBER94	3.48	2.16	3.43	2.94	3.34	3.36	3.10	3.70	3.49	3.29	3.47	3.03	2.49	3.30	2.62	4.00	2.59	4.47	3.25	4.31	3.29	0.56
AMBER96	3.11	4.83	5.71	5.40	5.53	5.76	5.27	5.66	5.33	5.15	5.28	5.00	4.38	5.71	5.38	6.08	3.84	5.63	5.43	5.35	5.19	0.68
AMBER99	2.05	1.85	2.73	2.27	2.47	2.49	2.56	2.77	2.48	2.25	2.55	2.17	1.65	2.68	1.77	3.42	2.46	4.17	2.32	2.76	2.50	0.55
AMBER99SB	2.39	2.64	2.98	2.84	2.64	3.43	2.40	2.86	2.70	2.60	2.68	2.59	2.50	2.89	2.81	3.39	1.83	2.92	3.02	3.14	2.76	0.35
AMBER03	3.90	3.96	5.66	4.53	5.51	6.76	4.51	4.77	4.65	4.24	4.09	4.77	5.17	6.48	3.79	7.89	3.95	6.25	4.75	4.71	5.02	1.07
CHARMM27	5.20	6.30	8.02	8.12	7.71	8.42	8.13	7.76	7.61	6.36	7.49	7.74	6.63	8.47	8.01	8.57	7.90	8.10	7.72	8.06	7.62	0.83
OPLS-AA	3.68	2.98	3.58	3.47	3.43	4.07	4.08	3.23	3.07	2.93	3.52	3.40	3.04	3.36	3.69	3.20	1.80	2.98	4.15	4.16	3.39	0.53
OPLS-AA/L	4.29	5.36	3.93	3.73	3.70	3.80	4.29	3.57	3.43	3.05	3.60	4.07	4.12	3.70	3.96	3.85	1.86	3.83	4.19	4.36	3.83	0.64
AMBERUA	21.63	4.89	6.12	4.54	5.95	5.26	5.13	5.87	5.84	5.49	5.48	5.55	4.58	6.97	5.20	6.79	4.69	5.73	4.92	4.92	6.28	3.58
GROMOS(G43b1)	18.24	4.53	4.94	4.39	4.59	4.61	5.23	5.01	4.78	4.78	4.65	5.41	4.59	4.29	5.38	4.80	7.33	5.43	4.74	6.48	5.71	2.96
GROMOS(G45a3)	17.67	4.24	4.40	4.25	4.11	4.21	4.82	4.58	4.31	4.25	4.10	4.97	4.13	4.17	4.92	4.38	5.19	5.46	3.93	5.01	5.16	2.90
GROMOS(G53a6)	18.42	5.54	5.74	5.56	5.53	5.58	4.86	5.65	5.40	5.33	5.21	5.53	5.07	5.57	5.82	6.13	5.39	5.04	5.11	5.26	6.09	2.84

[1] Standard deviation. [a] AMBER99 dispersion correction.

Table S3a. Energy offset (E_c, kcal/mol) for each tetrapeptide obtained from Eq. 2 in minimizing RMS of each method over 4 conformations (excluding α_L).

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg
M05-2X/cc-pVTZ	1.81	1.80	1.84	1.61	1.57	1.59	1.47	1.53	1.36	1.51	2.15	1.53	1.65	1.46	1.49	1.50	0.83	1.13	1.71	1.56
M05-2X-D[a]/cc-pVTZ	-2.33	-0.69	-0.61	-0.61	-0.53	-0.29	-0.56	-0.05	-0.24	0.07	-0.44	-0.79	-0.60	-0.59	-0.32	-0.80	-0.99	-1.37	0.10	0.18
M05-2X/6-31G**	0.36	0.28	0.39	0.22	0.00	0.16	-0.01	0.21	0.19	0.13	0.48	0.11	0.22	-0.12	0.16	-0.01	0.36	0.41	0.07	0.53
M05-2X-D[a]/6-31G**	-3.77	-2.22	-2.06	-2.00	-2.10	-1.72	-2.04	-1.37	-1.41	-1.31	-2.11	-2.22	-2.03	-2.17	-1.65	-2.31	-1.46	-2.10	-1.54	-0.84
PBE/cc-pVTZ	4.57	4.63	4.72	4.39	4.53	4.27	4.07	3.96	3.49	4.32	4.88	4.74	4.48	4.63	4.14	3.84	2.51	4.02	4.68	3.47
PBE-D[a]/cc-pVTZ	0.43	2.14	2.26	2.17	2.42	2.39	2.05	2.39	1.89	2.88	2.30	2.41	2.23	2.58	2.33	1.54	0.69	1.52	3.07	2.09
PBE/6-31G**	2.86	2.89	3.06	2.76	2.68	2.64	2.40	2.36	1.97	2.60	3.06	3.09	2.81	2.71	2.60	2.12	1.62	3.08	2.78	2.39
PBE-D[a]/6-31G**	-1.28	0.39	0.61	0.54	0.58	0.76	0.37	0.78	0.37	1.16	0.47	0.77	0.56	0.66	0.79	-0.18	-0.20	0.58	1.17	1.01
B3LYP/cc-pVTZ	5.44	5.51	5.71	5.28	5.52	5.23	4.95	4.85	4.42	5.21	5.99	5.74	5.55	5.64	5.10	4.73	2.82	4.43	5.71	4.20
B3LYP-D[a]/cc-pVTZ	1.30	3.01	3.26	3.06	3.41	3.35	2.92	3.27	2.82	3.76	3.40	3.42	3.30	3.59	3.28	2.44	1.00	1.92	4.09	2.83
B3LYP/6-31G**	3.70	3.67	3.99	3.58	3.59	3.50	3.24	3.14	2.68	3.37	4.01	4.04	3.85	3.65	3.49	2.97	1.99	3.24	3.72	3.04
B3LYP-D[a]/6-31G**	-0.44	1.17	1.54	1.36	1.49	1.63	1.21	1.56	1.08	1.93	1.42	1.72	1.60	1.60	1.68	0.68	0.17	0.74	2.11	1.67
AM1	3.71	4.12	3.77	3.10	4.10	3.16	2.17	3.95	3.50	4.04	4.68	3.49	2.46	2.70	2.47	1.83	1.94	3.87	3.72	0.13
AM1-D[a]	-0.42	1.62	1.32	0.88	2.00	1.28	0.14	2.37	1.90	2.60	2.10	1.16	0.21	0.65	0.66	-0.47	0.12	1.37	2.11	-1.25
PM3	8.81	7.57	8.25	8.04	9.17	7.97	6.78	7.78	7.50	8.22	8.77	7.70	6.20	9.45	6.45	6.23	7.24	7.84	8.15	4.46
PM3-D[a]	4.67	5.07	5.80	5.82	7.07	6.09	4.75	6.20	5.90	6.78	6.18	5.38	3.95	7.40	4.63	3.94	5.42	5.34	6.53	3.09
PM3MM	8.89	8.55	8.52	8.12	9.28	8.09	7.02	8.21	7.72	8.29	8.93	8.47	7.41	10.32	7.42	6.76	6.63	7.21	9.21	5.90
PM3MM-D[a]	4.75	6.06	6.07	5.90	7.17	6.21	4.99	6.63	6.12	6.85	6.34	6.15	5.16	8.27	5.60	4.46	4.81	4.71	7.60	4.53
AMOEBA	-3.17	0.44	0.73	0.03	0.23	-0.40	-0.14	-0.58	-0.68	2.61	0.37	1.80	-0.38	2.59	2.35	0.57	-0.87	-0.98	2.06	-0.35
AMBEREP	-3.66	0.39	-0.66	-0.24	-0.80	-0.44	-1.56	-1.24	-1.29	0.68	-2.07	-1.37	-0.83	-0.46	-0.49	-0.77	-1.15	-3.94	0.14	-1.45
AMBERPOL	-4.36	0.01	-1.01	-0.53	-1.12	-0.87	-1.91	-1.48	-1.64	-0.06	-2.35	-0.78	-0.83	-1.37	0.08	-0.94	-0.76	-3.88	-0.30	-2.14
AMBER94	-4.98	-1.79	-2.67	-2.26	-2.96	-1.74	-3.29	-3.22	-3.24	-3.15	-3.35	-2.89	-2.65	-2.85	-1.55	-3.22	-4.32	-5.81	-2.34	-3.94
AMBER96	1.10	4.30	3.41	3.82	3.12	4.34	2.79	2.86	2.84	2.93	2.73	3.19	3.43	3.23	4.53	2.87	1.76	0.27	3.74	2.14
AMBER99	-3.39	-0.56	-1.11	-0.69	-1.42	-0.14	-1.72	-1.65	-1.67	-1.58	-1.77	-1.32	-1.09	-1.27	-0.17	-1.81	-2.80	-4.25	-0.75	-2.40
AMBER99SB	2.00	3.70	3.96	4.39	3.64	4.97	3.33	3.39	3.37	3.51	3.27	3.75	3.99	4.39	4.74	3.08	2.19	0.82	4.31	2.65
AMBER03	0.38	2.33	2.32	3.31	2.06	4.72	1.12	0.99	-1.66	-1.84	-0.90	1.82	2.22	4.16	1.92	3.94	-0.61	1.87	5.83	0.59
CHARMM27	0.74	3.37	1.78	1.70	2.08	1.96	1.40	2.51	2.30	3.03	2.08	2.14	1.39	1.91	2.02	1.22	-4.04	-2.53	2.92	1.45
OPLS-AA	-0.15	3.63	3.84	3.86	4.21	4.44	2.93	4.48	4.24	4.10	2.90	4.60	4.15	4.51	5.37	3.20	0.73	0.84	5.83	2.82
OPLS-AA/L	-0.28	6.73	3.63	3.52	4.12	3.34	2.75	4.23	3.98	3.92	2.97	5.04	4.91	4.04	4.89	3.55	-1.64	-1.28	4.98	2.89
AMBERUA	0.82	2.54	0.67	1.93	0.21	0.83	0.19	0.25	-3.04	-0.37	-0.91	0.31	-0.71	1.55	2.12	1.41	-0.74	-0.12	0.52	-0.01
GROMOS(G43b1)	2.77	5.63	5.54	5.35	5.73	5.27	4.84	4.94	4.69	4.92	3.68	5.97	4.56	5.53	5.81	4.64	10.72	4.08	5.81	-2.77
GROMOS(G45a3)	3.49	5.87	5.83	5.50	5.87	5.21	4.99	5.33	4.94	5.06	3.99	6.22	4.79	5.65	6.05	4.73	4.76	2.30	5.41	0.82
GROMOS(G53a6)	0.71	7.89	7.86	7.42	8.24	7.24	6.01	7.43	7.04	6.79	6.18	7.92	6.90	7.50	7.40	6.72	5.10	4.36	7.30	3.86

[a] AMBER99 dispersion correction.

Table S3b. Signed error ($error = E_{ai} - E_{bi} + E_c$, kcal/mol) using the MP2 energy as the true value.

M05-2X/cc-pVTZ//M05-2X/6-31G**					M05-2X-D[a]/cc-pVTZ//M05-2X/6-31G**					M05-2X/6-31G**// M05-2X/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	1.81	-0.31	-0.54	-0.96	Pro	-2.33	1.47	2.80	-1.94	Pro	0.36	-0.31	-0.44	0.39
Gly	1.80	-0.36	-0.92	-0.52	Gly	-0.69	0.28	0.08	0.33	Gly	0.28	0.22	-0.67	0.17
Ala	1.84	-0.31	-0.86	-0.67	Ala	-0.61	0.48	0.04	0.08	Ala	0.39	0.17	-0.47	-0.10
Val	1.61	-0.24	-0.74	-0.63	Val	-0.61	0.11	0.07	0.43	Val	0.22	0.45	-0.45	-0.23
Leu	1.57	-0.20	-0.77	-0.60	Leu	-0.53	0.34	-0.02	0.21	Leu	0.00	0.51	-0.64	0.13
Ile	1.59	-0.24	-0.76	-0.59	Ile	-0.29	0.33	0.40	-0.44	Ile	0.16	0.44	-0.32	-0.27
Met	1.47	-0.34	-0.87	-0.27	Met	-0.56	0.41	-0.02	0.17	Met	-0.01	0.22	-0.51	0.30
Phe	1.53	-0.02	-0.06	-1.45	Phe	-0.05	-0.16	-0.05	0.25	Phe	0.21	0.16	0.15	-0.52
Tyr	1.36	0.00	0.17	-1.53	Tyr	-0.24	-0.27	0.15	0.35	Tyr	0.19	0.23	0.12	-0.54
His	1.51	-0.04	-0.20	-1.27	His	0.07	-0.50	0.04	0.40	His	0.13	0.08	0.07	-0.29
Trp	2.15	-0.92	0.06	-1.29	Trp	-0.44	0.68	-0.32	0.08	Trp	0.48	-0.47	0.40	-0.40
Cys	1.53	-0.32	-0.53	-0.68	Cys	-0.79	0.33	0.35	0.12	Cys	0.11	0.27	-0.37	0.00
Ser	1.65	-0.47	-0.80	-0.38	Ser	-0.60	0.43	0.19	-0.02	Ser	0.22	0.12	-0.50	0.16
Thr	1.46	-0.31	-0.65	-0.50	Thr	-0.59	0.34	0.23	0.02	Thr	-0.12	0.63	-0.33	-0.18
Asn	1.49	-0.72	-0.10	-0.67	Asn	-0.32	0.03	0.10	0.19	Asn	0.16	-0.51	0.29	0.06
Gln	1.50	-0.44	-0.90	-0.16	Gln	-0.80	0.65	0.24	-0.08	Gln	-0.01	0.11	-0.76	0.67
Asp	0.83	-0.44	-0.16	-0.22	Asp	-0.99	0.67	-0.44	0.76	Asp	0.36	-1.29	-0.31	1.23
Glu	1.13	0.49	-1.11	-0.52	Glu	-1.37	1.24	-0.20	0.33	Glu	0.41	-0.68	-0.28	0.55
Lys	1.71	-0.25	-0.66	-0.80	Lys	0.10	-0.73	0.48	0.15	Lys	0.07	0.48	-0.48	-0.08
Arg	1.56	-0.35	0.08	-1.28	Arg	0.18	-0.93	0.58	0.17	Arg	0.53	0.31	-0.70	-0.14

[a] AMBER99 dispersion correction.

M05-2X-D[a]/6-31G**// M05-2X/6-31G**					PBE/cc-pVTZ//PBE/6-31G**					PBE-D[a]/cc-pVTZ//PBE/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-3.77	1.47	2.89	-0.59	Pro	4.57	-2.36	-1.75	-0.46	Pro	0.43	-0.57	1.59	-1.44
Gly	-2.22	0.87	0.34	1.01	Gly	4.63	-2.57	-2.36	0.30	Gly	2.14	-1.93	-1.35	1.15
Ala	-2.06	0.97	0.44	0.65	Ala	4.72	-2.63	-2.55	0.46	Ala	2.26	-1.84	-1.64	1.21
Val	-2.00	0.81	0.36	0.84	Val	4.39	-2.55	-1.90	0.06	Val	2.17	-2.20	-1.10	1.13
Leu	-2.10	1.05	0.11	0.95	Leu	4.53	-2.43	-2.11	0.01	Leu	2.42	-1.89	-1.36	0.83
Ile	-1.72	1.01	0.83	-0.12	Ile	4.27	-2.54	-1.95	0.23	Ile	2.39	-1.98	-0.80	0.38
Met	-2.04	0.97	0.34	0.74	Met	4.07	-2.62	-2.40	0.94	Met	2.05	-1.87	-1.56	1.38
Phe	-1.37	0.02	0.16	1.19	Phe	3.96	-1.62	-1.03	-1.32	Phe	2.39	-1.76	-1.01	0.39
Tyr	-1.41	-0.03	0.10	1.34	Tyr	3.49	-1.08	-0.76	-1.65	Tyr	1.89	-1.35	-0.77	0.23
His	-1.31	-0.38	0.31	1.38	His	4.32	-1.57	-1.69	-1.07	His	2.88	-2.03	-1.45	0.59
Trp	-2.11	1.13	0.02	0.97	Trp	4.88	-2.80	-1.13	-0.96	Trp	2.30	-1.19	-1.51	0.40
Cys	-2.22	0.92	0.51	0.79	Cys	4.74	-3.83	-1.43	0.52	Cys	2.41	-3.18	-0.55	1.31
Ser	-2.03	1.02	0.49	0.52	Ser	4.48	-2.76	-2.13	0.41	Ser	2.23	-1.86	-1.14	0.77
Thr	-2.17	1.28	0.56	0.34	Thr	4.63	-2.57	-2.14	0.08	Thr	2.58	-1.92	-1.25	0.60
Asn	-1.65	0.24	0.49	0.93	Asn	4.14	-2.17	-1.77	-0.20	Asn	2.33	-1.42	-1.57	0.67
Gln	-2.31	1.20	0.37	0.74	Gln	3.84	-2.80	-2.36	1.33	Gln	1.54	-1.71	-1.22	1.40
Asp	-1.46	-0.17	-0.58	2.22	Asp	2.51	-1.21	-0.08	-1.22	Asp	0.69	-0.10	-0.36	-0.24
Glu	-2.10	0.07	0.62	1.40	Glu	4.02	-1.47	-2.27	-0.29	Glu	1.52	-0.73	-1.36	0.57
Lys	-1.54	0.00	0.67	0.87	Lys	4.68	-2.73	-2.04	0.09	Lys	3.07	-3.20	-0.90	1.03
Arg	-0.84	-0.27	-0.20	1.32	Arg	3.47	-2.61	-0.80	-0.06	Arg	2.09	-3.19	-0.30	1.40

PBE/6-31G**// PBE/6-31G**					PBE-D[a]/6-31G**// PBE/6-31G**					B3LYP/cc-pVTZ//B3LYP/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	2.86	-2.25	-1.52	0.91	Pro	-1.28	-0.47	1.82	-0.07	Pro	5.44	-2.20	-1.84	-1.40
Gly	2.89	-1.81	-1.95	0.87	Gly	0.39	-1.17	-0.95	1.72	Gly	5.51	-2.71	-2.23	-0.58
Ala	3.06	-1.88	-2.01	0.82	Ala	0.61	-1.09	-1.10	1.57	Ala	5.71	-2.67	-2.84	-0.20
Val	2.76	-1.60	-1.43	0.27	Val	0.54	-1.25	-0.63	1.34	Val	5.28	-2.68	-2.10	-0.50
Leu	2.68	-1.46	-1.79	0.58	Leu	0.58	-0.92	-1.05	1.39	Leu	5.52	-2.51	-2.29	-0.72
Ile	2.64	-1.60	-1.48	0.44	Ile	0.76	-1.04	-0.33	0.60	Ile	5.23	-2.65	-2.10	-0.47
Met	2.40	-1.76	-1.89	1.25	Met	0.37	-1.01	-1.05	1.69	Met	4.95	-2.77	-2.71	0.53
Phe	2.36	-1.16	-0.46	-0.75	Phe	0.78	-1.30	-0.44	0.96	Phe	4.85	-1.50	-1.19	-2.16
Tyr	1.97	-0.78	-0.16	-1.04	Tyr	0.37	-1.04	-0.17	0.84	Tyr	4.42	-1.08	-0.83	-2.51
His	2.60	-1.03	-1.12	-0.46	His	1.16	-1.49	-0.88	1.21	His	5.21	-1.43	-1.84	-1.94
Trp	3.06	-2.16	-0.50	-0.40	Trp	0.47	-0.55	-0.87	0.96	Trp	5.99	-2.91	-1.30	-1.79
Cys	3.09	-3.04	-1.09	1.04	Cys	0.77	-2.39	-0.21	1.83	Cys	5.74	-3.83	-1.63	-0.28
Ser	2.81	-1.97	-1.63	0.78	Ser	0.56	-1.07	-0.64	1.14	Ser	5.55	-2.98	-2.50	-0.06
Thr	2.71	-1.45	-1.60	0.34	Thr	0.66	-0.80	-0.71	0.86	Thr	5.64	-2.76	-2.33	-0.54
Asn	2.60	-1.69	-1.22	0.32	Asn	0.79	-0.94	-1.02	1.18	Asn	5.10	-2.34	-1.81	-0.95
Gln	2.12	-2.04	-2.01	1.94	Gln	-0.18	-0.95	-0.88	2.01	Gln	4.73	-2.92	-2.65	0.83
Asp	1.62	-2.18	0.36	0.20	Asp	-0.20	-1.06	0.08	1.18	Asp	2.82	-1.06	-0.19	-1.58
Glu	3.08	-2.26	-1.31	0.49	Glu	0.58	-1.52	-0.40	1.35	Glu	4.43	-0.46	-2.79	-1.18
Lys	2.78	-1.85	-1.60	0.67	Lys	1.17	-2.33	-0.46	1.62	Lys	5.71	-2.76	-2.23	-0.71
Arg	2.39	-1.55	-1.82	0.98	Arg	1.01	-2.13	-1.32	2.44	Arg	4.20	-2.76	-0.27	-1.17

[a] AMBER99 dispersion correction.

B3LYP-D[a]/cc-pVTZ//B3LYP/6-31G**					B3LYP/6-31G**// B3LYP/6-31G**					B3LYP-D[a]/6-31G**// B3LYP/6-31G**				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	1.30	-0.42	1.50	-2.38	Pro	3.70	-2.06	-1.61	-0.03	Pro	-0.44	-0.28	1.73	-1.01
Gly	3.01	-2.06	-1.22	0.27	Gly	3.67	-2.00	-1.72	0.05	Gly	1.17	-1.35	-0.71	0.90
Ala	3.26	-1.88	-1.93	0.55	Ala	3.99	-1.96	-2.31	0.28	Ala	1.54	-1.17	-1.41	1.03
Val	3.06	-2.33	-1.30	0.56	Val	3.58	-1.77	-1.64	-0.18	Val	1.36	-1.41	-0.83	0.89
Leu	3.41	-1.97	-1.54	0.10	Leu	3.59	-1.59	-1.97	-0.03	Leu	1.49	-1.05	-1.23	0.79
Ile	3.35	-2.08	-0.95	-0.32	Ile	3.50	-1.76	-1.65	-0.09	Ile	1.63	-1.20	-0.50	0.07
Met	2.92	-2.02	-1.87	0.97	Met	3.24	-1.95	-2.23	0.94	Met	1.21	-1.21	-1.38	1.38
Phe	3.27	-1.64	-1.17	-0.46	Phe	3.14	-1.03	-0.62	-1.49	Phe	1.56	-1.17	-0.60	0.22
Tyr	2.82	-1.34	-0.84	-0.63	Tyr	2.68	-0.48	-0.32	-1.88	Tyr	1.08	-0.75	-0.33	0.00
His	3.76	-1.89	-1.60	-0.27	His	3.37	-0.86	-1.30	-1.20	His	1.93	-1.32	-1.06	0.46
Trp	3.40	-1.30	-1.68	-0.42	Trp	4.01	-2.18	-0.72	-1.11	Trp	1.42	-0.58	-1.10	0.25
Cys	3.42	-3.18	-0.75	0.51	Cys	4.04	-3.07	-1.31	0.33	Cys	1.72	-2.41	-0.43	1.13
Ser	3.30	-2.08	-1.51	0.30	Ser	3.85	-2.23	-2.01	0.39	Ser	1.60	-1.33	-1.02	0.75
Thr	3.59	-2.11	-1.45	-0.03	Thr	3.65	-1.66	-1.79	-0.20	Thr	1.60	-1.02	-0.90	0.31
Asn	3.28	-1.59	-1.61	-0.09	Asn	3.49	-1.94	-1.27	-0.29	Asn	1.68	-1.19	-1.07	0.57
Gln	2.44	-1.83	-1.52	0.91	Gln	2.97	-2.19	-2.31	1.53	Gln	0.68	-1.10	-1.18	1.60
Asp	1.00	0.06	-0.46	-0.60	Asp	1.99	-2.00	0.04	-0.03	Asp	0.17	-0.89	-0.24	0.96
Glu	1.92	0.29	-1.89	-0.33	Glu	3.24	-1.20	-1.86	-0.18	Glu	0.74	-0.46	-0.95	0.67
Lys	4.09	-3.24	-1.09	0.24	Lys	3.72	-1.91	-1.79	-0.02	Lys	2.11	-2.39	-0.64	0.93
Arg	2.83	-3.34	0.23	0.28	Arg	3.04	-1.73	-1.24	-0.07	Arg	1.67	-2.31	-0.74	1.38

[a] AMBER99 dispersion correction.

AM1//AM1					AM1-D[a]// AM1					PM3// PM3				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	3.71	-2.93	-0.59	-0.19	Pro	-0.42	-1.15	2.75	-1.17	Pro	8.81	-3.01	-3.02	-2.78
Gly	4.12	-2.82	-0.34	-0.96	Gly	1.62	-2.18	0.67	-0.11	Gly	7.57	-1.35	-0.57	-5.64
Ala	3.77	-2.47	-0.28	-1.02	Ala	1.32	-1.68	0.63	-0.27	Ala	8.25	-2.43	-0.71	-5.11
Val	3.10	-2.15	0.51	-1.45	Val	0.88	-1.80	1.31	-0.39	Val	8.04	-2.57	-0.27	-5.21
Leu	4.10	-2.14	-0.30	-1.67	Leu	2.00	-1.60	0.45	-0.85	Leu	9.17	-2.54	-0.64	-5.99
Ile	3.16	-1.86	0.62	-1.92	Ile	1.28	-1.29	1.77	-1.77	Ile	7.97	-2.27	-0.32	-5.39
Met	2.17	-2.41	-0.13	0.37	Met	0.14	-1.66	0.71	0.81	Met	6.78	-2.49	-0.83	-3.46
Phe	3.95	-1.73	1.09	-3.32	Phe	2.37	-1.87	1.11	-1.61	Phe	7.78	-0.89	0.55	-7.44
Tyr	3.50	-1.27	1.45	-3.68	Tyr	1.90	-1.53	1.44	-1.80	Tyr	7.50	-0.94	1.06	-7.62
His	4.04	-1.68	0.51	-2.88	His	2.60	-2.14	0.75	-1.21	His	8.22	-1.57	-0.02	-6.63
Trp	4.68	-2.42	0.80	-3.07	Trp	2.10	-0.81	0.42	-1.70	Trp	8.77	-2.04	0.31	-7.03
Cys	3.49	-2.84	0.33	-0.98	Cys	1.16	-2.19	1.22	-0.18	Cys	7.70	-3.21	0.40	-4.89
Ser	2.46	-2.70	2.19	-1.95	Ser	0.21	-1.80	3.19	-1.59	Ser	6.20	-0.36	-1.02	-4.82
Thr	2.70	-2.29	0.08	-0.48	Thr	0.65	-1.64	0.96	0.03	Thr	9.45	-3.05	-1.64	-4.77
Asn	2.47	-0.51	-0.27	-1.69	Asn	0.66	0.24	-0.07	-0.82	Asn	6.45	-0.27	-0.48	-5.70
Gln	1.83	-2.78	-0.35	1.30	Gln	-0.47	-1.69	0.78	1.38	Gln	6.23	-2.96	-0.86	-2.41
Asp	1.94	0.86	-0.32	-2.49	Asp	0.12	1.98	-0.59	-1.50	Asp	7.24	1.89	-3.73	-5.40
Glu	3.87	0.92	-1.96	-2.82	Glu	1.37	1.66	-1.06	-1.97	Glu	7.84	0.95	-2.56	-6.23
Lys	3.72	-2.44	0.04	-1.33	Lys	2.11	-2.92	1.19	-0.38	Lys	8.15	-2.73	-0.31	-5.11
Arg	0.13	-3.98	6.26	-2.41	Arg	-1.25	-4.56	6.76	-0.96	Arg	4.46	-4.23	5.02	-5.25

[a] AMBER99 dispersion correction.

PM3-D[a]// PM3					PM3MM// PM3MM					PM3MM-D[a]// PM3MM				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	4.67	-1.23	0.31	-3.76	Pro	8.89	-3.46	-3.22	-2.21	Pro	4.75	-1.68	0.12	-3.19
Gly	5.07	-0.71	0.43	-4.79	Gly	8.55	-3.31	-1.04	-4.20	Gly	6.06	-2.66	-0.04	-3.36
Ala	5.80	-1.63	0.20	-4.36	Ala	8.52	-3.10	-1.24	-4.18	Ala	6.07	-2.30	-0.34	-3.43
Val	5.82	-2.22	0.54	-4.14	Val	8.12	-3.12	-0.60	-4.40	Val	5.90	-2.76	0.20	-3.33
Leu	7.07	-2.01	0.10	-5.17	Leu	9.28	-3.20	-0.99	-5.10	Leu	7.17	-2.66	-0.24	-4.28
Ile	6.09	-1.70	0.84	-5.23	Ile	8.09	-2.89	-0.68	-4.51	Ile	6.21	-2.33	0.47	-4.36
Met	4.75	-1.75	0.01	-3.02	Met	7.02	-3.19	-1.32	-2.50	Met	4.99	-2.45	-0.47	-2.06
Phe	6.20	-1.03	0.56	-5.74	Phe	8.21	-2.15	0.43	-6.49	Phe	6.63	-2.29	0.45	-4.78
Tyr	5.90	-1.20	1.05	-5.75	Tyr	7.72	-1.66	0.81	-6.87	Tyr	6.12	-1.93	0.80	-5.00
His	6.78	-2.03	0.22	-4.96	His	8.29	-2.04	-0.20	-6.05	His	6.85	-2.51	0.04	-4.38
Trp	6.18	-0.44	-0.07	-5.66	Trp	8.93	-2.82	0.23	-6.34	Trp	6.34	-1.21	-0.15	-4.98
Cys	5.38	-2.56	1.28	-4.10	Cys	8.47	-3.65	-1.02	-3.80	Cys	6.15	-2.99	-0.14	-3.01
Ser	3.95	0.54	-0.03	-4.46	Ser	7.41	-3.64	1.11	-4.89	Ser	5.16	-2.74	2.10	-4.53
Thr	7.40	-2.40	-0.75	-4.25	Thr	10.32	-3.46	-3.86	-2.99	Thr	8.27	-2.81	-2.98	-2.48
Asn	4.63	0.47	-0.28	-4.83	Asn	7.42	-1.72	-0.88	-4.81	Asn	5.60	-0.97	-0.68	-3.95
Gln	3.94	-1.87	0.27	-2.33	Gln	6.76	-3.55	-1.60	-1.61	Gln	4.46	-2.46	-0.47	-1.54
Asp	5.42	3.00	-4.00	-4.42	Asp	6.63	2.43	-2.96	-6.10	Asp	4.81	3.54	-3.23	-5.12
Glu	5.34	1.70	-1.66	-5.38	Glu	7.21	0.74	-2.53	-5.42	Glu	4.71	1.49	-1.63	-4.57
Lys	6.53	-3.21	0.83	-4.16	Lys	9.21	-3.70	-1.12	-4.39	Lys	7.60	-4.18	0.03	-3.45
Arg	3.09	-4.81	5.52	-3.79	Arg	5.90	-5.25	4.10	-4.75	Arg	4.53	-5.83	4.60	-3.30

[a] AMBER99 dispersion correction.

AMOEBA// AMOEBA					AMBEREP// AMBEREP					AMBERPOL// AMBERPOL				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-3.17	1.98	5.24	-4.06	Pro	-3.66	2.73	2.54	-1.61	Pro	-4.36	3.62	3.87	-3.14
Gly	0.44	0.26	0.64	-1.34	Gly	0.39	-0.70	-1.56	1.88	Gly	0.01	0.42	0.56	-0.99
Ala	0.73	0.29	0.14	-1.16	Ala	-0.66	0.48	-0.63	0.82	Ala	-1.01	1.40	0.72	-1.10
Val	0.03	0.85	1.64	-2.52	Val	-0.24	0.22	-0.44	0.47	Val	-0.53	0.90	0.79	-1.16
Leu	0.23	-0.01	1.06	-1.28	Leu	-0.80	0.94	-0.86	0.73	Leu	-1.12	1.73	0.33	-0.94
Ile	-0.40	0.46	1.29	-1.36	Ile	-0.44	0.63	-0.29	0.10	Ile	-0.87	1.49	1.03	-1.65
Met	-0.14	0.54	0.09	-0.48	Met	-1.56	0.50	-0.73	1.79	Met	-1.91	1.29	0.58	0.04
Phe	-0.58	0.46	1.23	-1.11	Phe	-1.24	0.74	0.46	0.05	Phe	-1.48	1.40	1.60	-1.52
Tyr	-0.68	0.61	1.33	-1.26	Tyr	-1.29	0.77	0.35	0.16	Tyr	-1.64	1.57	1.84	-1.77
His	2.61	-0.21	-0.33	-2.08	His	0.68	-0.43	0.11	-0.37	His	-0.06	0.60	1.12	-1.66
Trp	0.37	0.70	1.22	-2.29	Trp	-2.07	1.40	0.64	0.03	Trp	-2.35	2.24	1.75	-1.63
Cys	1.80	-1.71	0.94	-1.03	Cys	-1.37	1.47	0.46	-0.57	Cys	-0.78	1.28	0.86	-1.36
Ser	-0.38	0.31	0.00	0.08	Ser	-0.83	0.46	-0.70	1.07	Ser	-0.83	1.06	0.35	-0.58
Thr	2.59	-0.03	0.60	-3.16	Thr	-0.46	1.21	0.64	-1.38	Thr	-1.37	1.46	1.42	-1.51
Asn	2.35	0.12	-2.38	-0.08	Asn	-0.49	1.66	-2.37	1.19	Asn	0.08	1.77	-1.50	-0.35
Gln	0.57	-0.41	-0.26	0.11	Gln	-0.77	0.75	-0.11	0.13	Gln	-0.94	1.43	1.07	-1.55
Asp	-0.87	3.96	-0.90	-2.19	Asp	-1.15	1.70	-1.89	1.34	Asp	-0.76	2.19	-1.04	-0.38
Glu	-0.98	2.63	1.04	-2.69	Glu	-3.94	3.48	-1.13	1.58	Glu	-3.88	4.07	0.16	-0.35
Lys	2.06	-0.77	0.66	-1.96	Lys	0.14	-0.13	-0.45	0.43	Lys	-0.30	0.12	1.01	-0.83
Arg	-0.35	0.72	0.86	-1.23	Arg	-1.45	-0.99	2.78	-0.34	Arg	-2.14	-0.24	3.83	-1.45

AMBER94// AMBER94					AMBER96// AMBER96					AMBER99// AMBER99				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-4.98	1.83	5.19	-2.04	Pro	1.10	-0.65	1.30	-1.75	Pro	-3.39	2.23	1.90	-0.74
Gly	-1.79	0.85	1.58	-0.65	Gly	4.30	-1.62	-2.31	-0.36	Gly	-0.56	1.65	-1.58	0.50
Ala	-2.67	1.81	1.80	-0.94	Ala	3.41	-0.67	-2.09	-0.65	Ala	-1.11	2.20	-1.45	0.36
Val	-2.26	1.31	1.71	-0.76	Val	3.82	-1.17	-2.18	-0.47	Val	-0.69	1.69	-1.54	0.53
Leu	-2.96	0.86	2.44	-0.34	Leu	3.12	-1.62	-1.46	-0.05	Leu	-1.42	1.22	-0.76	0.95
Ile	-1.74	1.73	2.18	-2.17	Ile	4.34	-0.75	-1.71	-1.88	Ile	-0.14	2.10	-1.09	-0.88
Met	-3.29	1.69	1.35	0.25	Met	2.79	-0.79	-2.54	0.54	Met	-1.72	2.07	-1.91	1.55
Phe	-3.22	1.78	2.71	-1.27	Phe	2.86	-0.69	-1.19	-0.98	Phe	-1.65	2.18	-0.55	0.02
Tyr	-3.24	1.88	2.91	-1.56	Tyr	2.84	-0.59	-0.98	-1.27	Tyr	-1.67	2.27	-0.34	-0.27
His	-3.15	1.64	2.91	-1.40	His	2.93	-0.84	-0.98	-1.11	His	-1.58	2.02	-0.34	-0.10
Trp	-3.35	2.30	2.55	-1.50	Trp	2.73	-0.18	-1.34	-1.21	Trp	-1.77	2.68	-0.70	-0.21
Cys	-2.89	2.13	2.26	-1.49	Cys	3.19	-0.35	-1.64	-1.20	Cys	-1.32	2.52	-0.99	-0.21
Ser	-2.65	2.16	2.16	-1.67	Ser	3.43	-0.32	-1.73	-1.38	Ser	-1.09	2.55	-1.09	-0.37
Thr	-2.85	0.90	1.53	0.42	Thr	3.23	-1.58	-2.36	0.71	Thr	-1.27	1.29	-1.73	1.71
Asn	-1.55	0.15	1.93	-0.53	Asn	4.53	-2.33	-1.96	-0.24	Asn	-0.17	0.34	-0.75	0.59
Gln	-3.22	2.11	2.17	-1.06	Gln	2.87	-0.37	-1.72	-0.78	Gln	-1.81	2.35	-1.25	0.71
Asp	-4.32	2.93	0.78	0.62	Asp	1.76	0.45	-3.11	0.90	Asp	-2.80	3.47	-2.52	1.85
Glu	-5.81	5.01	0.48	0.31	Glu	0.27	2.54	-3.41	0.60	Glu	-4.25	5.40	-2.77	1.61
Lys	-2.34	1.52	2.64	-1.82	Lys	3.74	-0.96	-1.25	-1.53	Lys	-0.75	1.90	-0.62	-0.53
Arg	-3.94	0.70	6.04	-2.80	Arg	2.14	-1.78	2.15	-2.51	Arg	-2.40	1.04	2.94	-1.57

AMBER99SB// AMBER99SB					AMBER03// AMBER03					CHARMM27// CHARMM27				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	2.00	1.51	0.60	-4.10	Pro	0.38	3.18	0.24	-3.80	Pro	0.74	1.24	2.15	-4.12
Gly	3.70	0.28	-1.07	-2.92	Gly	2.33	0.16	-0.37	-2.12	Gly	3.37	-1.97	-0.64	-0.76
Ala	3.96	0.43	-1.64	-2.75	Ala	2.32	0.84	-0.93	-2.23	Ala	1.78	-0.38	0.63	-2.03
Val	4.39	-0.06	-1.72	-2.60	Val	3.31	-0.22	-1.67	-1.42	Val	1.70	-0.80	1.23	-2.13
Leu	3.64	-0.55	-0.95	-2.14	Leu	2.06	0.23	-0.08	-2.22	Leu	2.08	-0.96	1.34	-2.46
Ile	4.97	0.38	-1.23	-4.12	Ile	4.72	-0.04	-1.39	-3.28	Ile	1.96	-0.52	1.50	-2.94
Met	3.33	0.29	-2.09	-1.53	Met	1.12	1.23	-0.83	-1.53	Met	1.40	-0.50	0.24	-1.14
Phe	3.39	0.40	-0.73	-3.06	Phe	0.99	1.16	0.45	-2.60	Phe	2.51	-0.58	1.46	-3.38
Tyr	3.37	0.50	-0.49	-3.38	Tyr	-1.66	2.26	1.68	-2.29	Tyr	2.30	-0.37	1.69	-3.62
His	3.51	0.27	-0.49	-3.28	His	-1.84	2.27	1.81	-2.24	His	3.03	-0.56	1.31	-3.78
Trp	3.27	0.89	-0.85	-3.32	Trp	-0.90	1.37	1.16	-1.63	Trp	2.08	-0.77	1.47	-2.78
Cys	3.75	0.60	-1.14	-3.21	Cys	1.82	1.26	-0.21	-2.87	Cys	2.14	-0.51	1.12	-2.75
Ser	3.99	0.76	-1.29	-3.46	Ser	2.22	1.05	-0.88	-2.38	Ser	1.39	-1.06	-0.04	-0.29
Thr	4.39	-0.48	-1.93	-1.98	Thr	4.16	0.00	-0.22	-3.95	Thr	1.91	-1.37	0.80	-1.33
Asn	4.74	-1.48	-0.71	-2.54	Asn	1.92	-0.66	0.40	-1.66	Asn	2.02	1.12	-0.43	-2.70
Gln	3.08	0.43	-1.59	-1.92	Gln	3.94	0.11	-1.96	-2.09	Gln	1.22	-0.46	0.67	-1.44
Asp	2.19	1.74	-2.67	-1.27	Asp	-0.61	2.83	-2.46	0.24	Asp	-4.04	6.35	0.50	-2.80
Glu	0.82	3.66	-2.95	-1.53	Glu	1.87	3.77	-3.81	-1.83	Glu	-2.53	3.77	0.76	-2.00
Lys	4.31	0.15	-0.80	-3.65	Lys	5.83	-0.47	-0.33	-5.04	Lys	2.92	-1.24	1.06	-2.74
Arg	2.65	-0.74	2.81	-4.72	Arg	0.59	-0.95	5.96	-5.60	Arg	1.45	-2.12	5.00	-4.33

OPLS-AA// OPLS-AA					OPLS-AA/L// OPLS-AA/L					AMBERUA// AMBERUA				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	-0.15	-1.32	6.41	-4.94	Pro	-0.28	-0.32	7.01	-6.41	Pro	0.82	1.51	2.12	-4.45
Gly	3.63	-1.70	-1.21	-0.72	Gly	6.73	-3.60	-3.12	-0.01	Gly	2.54	0.07	-0.66	-1.94
Ala	3.84	-1.67	-1.17	-1.00	Ala	3.63	-0.31	-1.27	-2.04	Ala	0.67	1.49	-0.32	-1.83
Val	3.86	-1.69	-0.63	-1.55	Val	3.52	-0.40	-0.85	-2.26	Val	1.93	1.25	0.00	-3.17
Leu	4.21	-2.12	-0.74	-1.35	Leu	4.12	-0.56	-0.88	-2.68	Leu	0.21	1.21	0.22	-1.64
Ile	4.44	-1.18	-0.09	-3.17	Ile	3.34	-0.64	-1.03	-1.68	Ile	0.83	1.54	0.20	-2.57
Met	2.93	-2.58	-2.38	2.03	Met	2.75	-1.30	-2.48	1.02	Met	0.19	1.30	-0.40	-1.09
Phe	4.48	-1.88	-0.08	-2.52	Phe	4.23	-0.56	0.00	-3.67	Phe	0.25	1.68	0.75	-2.68
Tyr	4.24	-1.64	0.17	-2.77	Tyr	3.98	-0.36	0.29	-3.92	Tyr	-3.04	2.88	2.08	-1.92
His	4.10	-1.63	-0.23	-2.25	His	3.92	-0.47	-0.17	-3.27	His	-0.37	1.92	1.05	-2.59
Trp	2.90	-2.94	1.05	-1.01	Trp	2.97	-1.35	0.75	-2.36	Trp	-0.91	2.10	1.19	-2.38
Cys	4.60	-2.52	-1.13	-0.95	Cys	5.04	-1.77	-1.94	-1.32	Cys	0.31	1.69	0.33	-2.33
Ser	4.15	-2.19	-1.59	-0.36	Ser	4.91	0.19	-1.02	-4.08	Ser	-0.71	1.16	-0.48	0.03
Thr	4.51	-1.52	-0.24	-2.75	Thr	4.04	-0.33	-0.31	-3.40	Thr	1.55	-0.04	-1.19	-0.32
Asn	5.37	-5.16	-0.08	-0.13	Asn	4.89	-0.78	-2.35	-1.76	Asn	2.12	-0.51	0.27	-1.88
Gln	3.20	-0.36	0.10	-2.94	Gln	3.55	-0.27	-0.75	-2.54	Gln	1.41	1.67	-0.18	-2.90
Asp	0.73	-3.06	2.36	-0.02	Asp	-1.64	2.10	1.40	-1.86	Asp	-0.74	2.20	-0.66	-0.80
Glu	0.84	3.05	-2.05	-1.84	Glu	-1.28	2.64	-0.28	-1.08	Glu	-0.12	4.16	-2.23	-1.82
Lys	5.83	-2.76	-1.17	-1.90	Lys	4.98	-1.27	-1.00	-2.70	Lys	0.52	1.17	0.60	-2.29
Arg	2.82	-3.31	3.96	-3.48	Arg	2.89	-1.98	3.68	-4.59	Arg	-0.01	-0.66	5.18	-4.51

GROMOS(G43b1)// GROMOS(G43b1)					GROMOS(G45a3)// GROMOS(G45a3)					GROMOS(G53a6)// GROMOS(G53a6)				
	α_R	β	β_a	PPII		α_R	β	β_a	PPII		α_R	β	β_a	PPII
Pro	2.77	-1.27	1.90	-3.40	Pro	3.49	-1.64	1.44	-3.29	Pro	0.71	-4.21	11.21	-7.71
Gly	5.63	-3.81	-1.11	-0.71	Gly	5.87	-4.00	-1.29	-0.58	Gly	7.89	-4.81	-2.59	-0.49
Ala	5.54	-3.64	-1.24	-0.66	Ala	5.83	-3.92	-1.49	-0.42	Ala	7.86	-4.72	-2.76	-0.38
Val	5.35	-3.44	-0.28	-1.63	Val	5.50	-3.69	-0.37	-1.44	Val	7.42	-4.65	-1.54	-1.23
Leu	5.73	-3.69	-1.20	-0.84	Leu	5.87	-4.29	-1.05	-0.54	Leu	8.24	-4.93	-1.94	-1.37
Ile	5.27	-3.41	-0.29	-1.57	Ile	5.21	-3.80	-0.40	-1.02	Ile	7.24	-4.64	-1.44	-1.16
Met	4.84	-3.66	-1.20	0.02	Met	4.99	-3.96	-1.39	0.36	Met	6.01	-4.39	-2.33	0.70
Phe	4.94	-3.29	-0.63	-1.02	Phe	5.33	-3.61	-0.84	-0.88	Phe	7.43	-4.46	-1.77	-1.21
Tyr	4.69	-2.94	-0.86	-0.88	Tyr	4.94	-3.34	-0.85	-0.76	Tyr	7.04	-4.18	-1.79	-1.07
His	4.92	-2.58	-0.42	-1.93	His	5.06	-3.03	-0.06	-1.97	His	6.79	-4.69	-0.81	-1.29
Trp	3.68	-1.96	-0.25	-1.47	Trp	3.99	-2.13	-0.41	-1.45	Trp	6.18	-3.07	-1.11	-2.00
Cys	5.97	-3.66	-0.72	-1.59	Cys	6.22	-3.93	-0.89	-1.40	Cys	7.92	-4.63	-2.39	-0.90
Ser	4.56	-3.47	-0.93	-0.16	Ser	4.79	-3.74	-1.12	0.07	Ser	6.90	-3.90	-1.91	-1.09
Thr	5.53	-3.43	-1.05	-1.05	Thr	5.65	-3.84	-1.21	-0.59	Thr	7.50	-3.90	-1.27	-2.33
Asn	5.81	-2.30	-2.33	-1.17	Asn	6.05	-2.51	-2.54	-1.00	Asn	7.40	-4.09	-1.89	-1.42
Gln	4.64	-2.99	-0.32	-1.32	Gln	4.73	-3.46	-0.60	-0.67	Gln	6.72	-3.74	-1.41	-1.57
Asp	10.72	2.84	-3.51	-10.04	Asp	4.76	5.53	-3.78	-6.50	Asp	5.10	3.56	-3.95	-4.71
Glu	4.08	6.78	-4.06	-6.80	Glu	2.30	8.07	-4.40	-5.97	Glu	4.36	4.99	-5.01	-4.34
Lys	5.81	-5.17	-1.14	0.50	Lys	5.41	-5.30	-0.61	0.50	Lys	7.30	-5.55	-1.61	-0.14
Arg	-2.77	-6.37	10.19	-1.04	Arg	0.82	-6.91	7.89	-1.79	Arg	3.86	-7.30	5.81	-2.37

Table S3c. Signed RMS-C excluding α_L (RMS-C-Nα_L, kcal/mol) of each conformation over 20 amino acids for each method.

	α_R	β	β_a	PPII	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.58	-0.40	-0.64	-0.85	0.87	0.44
M05-2X-D[a]/cc-pVTZ	-0.79	0.63	0.68	0.52	0.66	0.10
M05-2X/6-31G**	0.27	0.47	-0.45	0.42	0.40	0.08
M05-2X-D[a]/6-31G**	-2.01	0.84	0.78	1.04	1.17	0.49
PBE/cc-pVTZ	4.25	-2.43	-1.85	-0.77	2.33	1.26
PBE-D[a]/cc-pVTZ	2.18	-1.96	-1.21	0.95	1.57	0.51
PBE/6-31G**	2.65	-1.84	-1.46	0.83	1.70	0.66
PBE-D[a]/6-31G**	0.73	-1.33	-0.86	1.40	1.08	0.29
B3LYP/cc-pVTZ	5.15	-2.48	-2.03	-1.21	2.72	1.48
B3LYP-D[a]/cc-pVTZ	3.07	-2.02	-1.38	-0.71	1.80	0.87
B3LYP/6-31G**	3.46	-1.86	-1.61	-0.78	1.93	0.97
B3LYP-D[a]/6-31G**	1.42	-1.35	-0.98	0.88	1.16	0.23
AM1	3.32	-2.31	1.64	-2.05	2.33	0.62
AM1-D[a]	1.45	-2.00	2.00	-1.20	1.66	0.35
PM3	7.71	-2.32	-1.78	-5.51	4.33	2.42
PM3-D[a]	5.61	-2.10	1.66	-4.60	3.49	1.66
PM3MM	8.11	-3.10	-1.89	-4.79	4.47	2.34
PM3MM-D[a]	6.01	-2.79	-1.58	-3.88	3.56	1.63
AMOEBA	1.43	1.29	1.56	-1.88	1.54	0.22
AMBEREP	-1.55	1.35	-1.25	1.01	1.29	0.19
AMBERPOL	-1.74	1.79	1.60	-1.38	1.63	0.16
AMBER94	-3.28	2.02	2.68	-1.37	2.34	0.71
AMBER96	3.14	-1.21	-1.98	-1.17	1.87	0.80
AMBER99	-1.87	2.38	-1.54	0.95	1.68	0.52
AMBER99SB	3.60	1.12	-1.58	-3.02	2.33	1.02
AMBER03	2.65	1.62	-1.94	-2.83	2.26	0.50
CHARMM27	2.26	-1.93	1.57	-2.70	2.11	0.42
OPLS-AA	3.83	-2.43	2.03	-2.24	2.63	0.70
OPLS-AA/L	3.90	-1.40	-2.21	-2.99	2.62	0.93
AMBERUA	1.28	1.76	1.54	-2.43	1.75	0.43
GROMOS(G43b1)	5.39	-3.76	-2.76	-3.01	3.73	1.03
GROMOS(G45a3)	5.01	-4.29	-2.42	-2.32	3.51	1.17
GROMOS(G53a6)	6.73	-4.60	-3.57	-2.57	4.37	1.54

[1] Standard deviation. [a] AMBER99 dispersion correction.

Table S3d. RMS over the four conformations (RMS-Nα_L, kcal/mol) of each amino acid for each method.

	Pro	Gly	Ala	Val	Leu	Ile	Met	Phe	Tyr	His	Trp	Cys	Ser	Thr	Asn	Gln	Asp	Glu	Lys	Arg	Mean(μ)	[1]SD(σ)
M05-2X/cc-pVTZ	1.07	1.06	1.08	0.95	0.93	0.94	0.88	1.06	1.03	0.99	1.33	0.89	0.96	0.85	0.90	0.91	0.49	0.87	1.01	1.03	0.96	0.15
M05-2X-D[a]/cc-pVTZ	2.19	0.41	0.39	0.38	0.33	0.37	0.35	0.15	0.26	0.32	0.44	0.47	0.38	0.36	0.19	0.53	0.74	0.94	0.45	0.56	0.51	0.42
M05-2X/6-31G**	0.38	0.39	0.32	0.36	0.41	0.32	0.31	0.30	0.31	0.17	0.44	0.23	0.29	0.37	0.31	0.51	0.92	0.50	0.34	0.47	0.38	0.15
M05-2X-D[a]/6-31G**	2.51	1.30	1.20	1.17	1.27	1.08	1.20	0.91	0.97	0.98	1.29	1.29	1.19	1.30	0.99	1.36	1.36	1.30	0.95	0.80	1.22	0.34
PBE/cc-pVTZ	2.72	2.90	3.00	2.71	2.78	2.67	2.74	2.30	2.04	2.51	2.91	3.14	2.85	2.86	2.50	2.73	1.52	2.43	2.89	2.21	2.62	0.37
PBE-D[a]/cc-pVTZ	1.13	1.69	1.78	1.73	1.73	1.61	1.73	1.58	1.23	1.93	1.51	2.12	1.61	1.75	1.61	1.48	0.41	1.12	2.32	2.04	1.61	0.40
PBE/6-31G**	2.02	2.01	2.10	1.75	1.79	1.73	1.87	1.39	1.18	1.52	1.90	2.30	1.94	1.74	1.67	2.03	1.37	2.03	1.88	1.76	1.80	0.27
PBE-D[a]/6-31G**	1.14	1.16	1.14	1.00	1.03	0.73	1.13	0.92	0.70	1.20	0.74	1.56	0.89	0.76	0.99	1.20	0.80	1.07	1.55	1.82	1.08	0.29
B3LYP/cc-pVTZ	3.15	3.28	3.46	3.15	3.26	3.12	3.16	2.82	2.63	3.01	3.51	3.55	3.39	3.36	2.98	3.11	1.70	2.69	3.38	2.59	3.07	0.42
B3LYP-D[a]/cc-pVTZ	1.56	1.93	2.13	2.05	2.12	2.03	2.07	1.93	1.65	2.26	2.02	2.38	2.10	2.20	1.99	1.76	0.63	1.36	2.67	2.20	1.95	0.41
B3LYP/6-31G**	2.27	2.26	2.51	2.16	2.20	2.13	2.24	1.84	1.66	1.95	2.38	2.63	2.45	2.20	2.10	2.31	1.41	1.97	2.28	1.86	2.14	0.28
B3LYP-D[a]/6-31G**	1.04	1.06	1.30	1.16	1.17	1.04	1.30	1.03	0.68	1.31	0.95	1.60	1.22	1.06	1.19	1.18	0.67	0.73	1.69	1.63	1.15	0.28
AM1	2.39	2.55	2.32	2.04	2.46	2.09	1.63	2.78	2.72	2.63	3.07	2.31	2.34	1.79	1.52	1.80	1.64	2.63	2.32	3.90	2.35	0.55
AM1-D[a]	1.61	1.40	1.12	1.21	1.37	1.55	0.99	1.80	1.68	1.83	1.43	1.38	2.00	1.01	0.54	1.18	1.28	1.55	1.90	4.15	1.55	0.69
PM3	5.09	4.77	5.02	4.96	5.63	4.95	4.03	5.41	5.39	5.34	5.71	4.84	3.96	5.57	4.31	3.68	4.97	5.19	5.00	4.76	4.93	0.55
PM3-D[a]	3.06	3.51	3.72	3.75	4.49	4.13	2.95	4.27	4.19	4.32	4.20	3.67	2.99	4.45	3.36	2.48	4.30	3.97	4.21	4.40	3.82	0.57
PM3MM	5.15	5.07	5.03	4.88	5.55	4.86	4.11	5.34	5.25	5.23	5.65	5.01	4.83	5.97	4.52	3.98	4.89	4.70	5.46	5.05	5.03	0.47
PM3MM-D[a]	2.98	3.71	3.67	3.66	4.38	3.97	2.97	4.25	4.09	4.25	4.08	3.74	3.84	4.78	3.48	2.67	4.25	3.46	4.67	4.65	3.88	0.56
AMOEBA	3.81	0.79	0.70	1.56	0.84	0.98	0.37	0.91	1.02	1.68	1.36	1.42	0.25	2.07	1.67	0.38	2.35	2.01	1.51	0.85	1.33	0.81
AMBEREP	2.74	1.29	0.66	0.36	0.83	0.42	1.27	0.76	0.77	0.45	1.29	1.07	0.80	1.00	1.58	0.55	1.55	2.80	0.33	1.65	1.11	0.68
AMBERPOL	3.77	0.61	1.08	0.87	1.15	1.30	1.19	1.50	1.71	1.05	2.01	1.10	0.75	1.44	1.17	1.27	1.28	2.82	0.67	2.31	1.45	0.75
AMBER94	3.85	1.31	1.91	1.61	1.97	1.97	1.97	2.37	2.50	2.40	2.51	2.25	2.19	1.69	1.27	2.27	2.66	3.85	2.12	3.89	2.33	0.74
AMBER96	1.26	2.58	2.05	2.29	1.90	2.54	1.95	1.66	1.66	1.69	1.64	1.90	2.05	2.18	2.73	1.73	1.86	2.15	2.17	2.16	2.01	0.35
AMBER99	2.27	1.20	1.44	1.22	1.12	1.27	1.82	1.39	1.43	1.30	1.65	1.51	1.50	1.52	0.51	1.65	2.72	3.79	1.10	2.12	1.63	0.67
AMBER99SB	2.42	2.42	2.55	2.69	2.18	3.29	2.12	2.32	2.41	2.42	2.41	2.55	2.75	2.60	2.81	1.99	2.04	2.50	2.85	3.07	2.52	0.32
AMBER03	2.49	1.59	1.73	1.99	1.52	2.96	1.20	1.53	1.99	2.05	1.29	1.82	1.77	2.87	1.33	2.44	1.90	2.98	3.86	4.13	2.17	0.80
CHARMM27	2.43	2.01	1.40	1.55	1.81	1.93	0.94	2.25	2.31	2.52	1.92	1.85	0.89	1.41	1.79	1.03	4.02	2.51	2.16	3.55	2.01	0.77
OPLS-AA	4.10	2.12	2.23	2.27	2.48	2.79	2.50	2.74	2.66	2.48	2.19	2.72	2.48	2.75	3.72	2.18	1.97	2.10	3.41	3.42	2.67	0.57
OPLS-AA/L	4.75	4.12	2.18	2.14	2.51	1.96	2.03	2.81	2.80	2.56	2.05	2.92	3.23	2.65	2.88	2.22	1.77	1.57	2.95	3.42	2.68	0.76
AMBERUA	2.61	1.63	1.24	1.96	1.03	1.56	0.87	1.63	2.53	1.71	1.76	1.46	0.72	0.99	1.44	1.82	1.27	2.53	1.34	3.45	1.68	0.66
GROMOS(G43b1)	2.47	3.46	3.39	3.28	3.48	3.24	3.09	3.03	2.84	2.95	2.21	3.61	2.90	3.34	3.39	2.84	7.68	5.60	3.94	6.19	3.65	1.30
GROMOS(G45a3)	2.64	3.62	3.60	3.40	3.68	3.27	3.26	3.28	3.03	3.11	2.39	3.77	3.09	3.48	3.55	2.96	5.24	5.60	3.81	5.33	3.61	0.83
GROMOS(G53a6)	7.13	4.81	4.79	4.49	4.95	4.40	3.91	4.46	4.23	4.19	3.64	4.76	4.11	4.43	4.39	3.99	4.37	4.69	4.66	5.19	4.58	0.69

[1] Standard deviation. [a] AMBER99 dispersion correction.

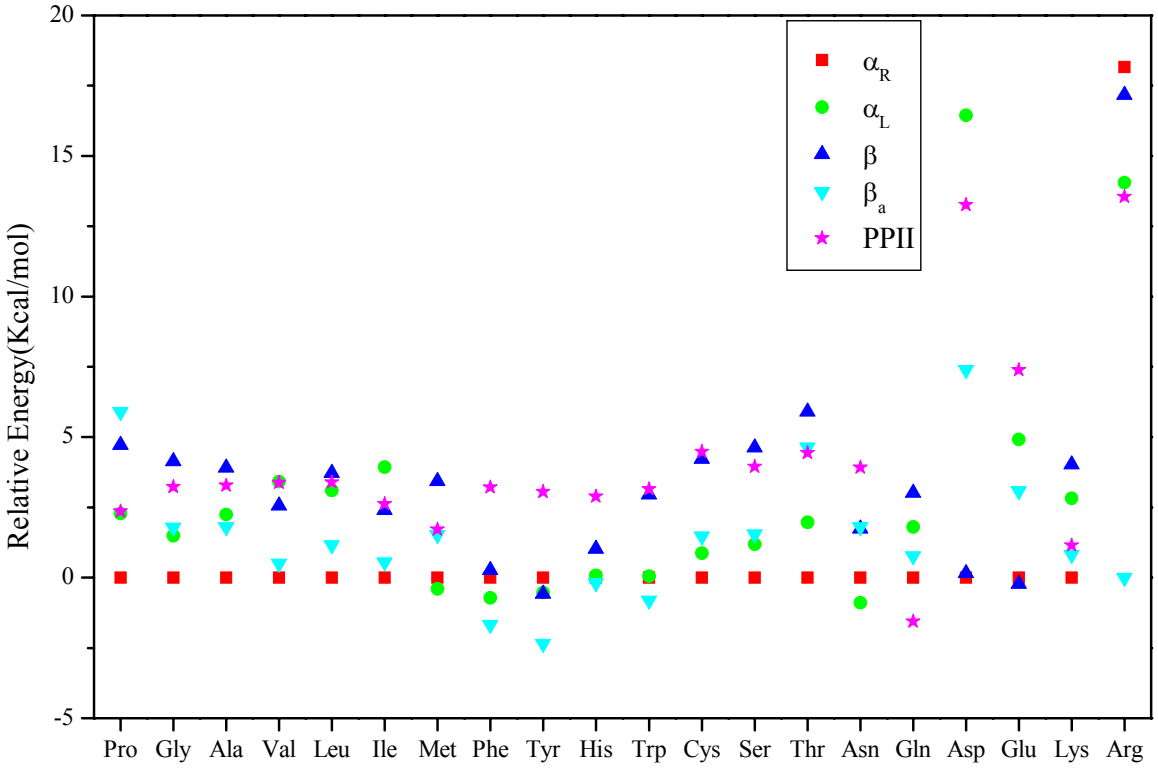

Figure S1. Relative energies of five conformations of 20 amino acids using MP2/cc-pVTZ//M052x/6-31G**.

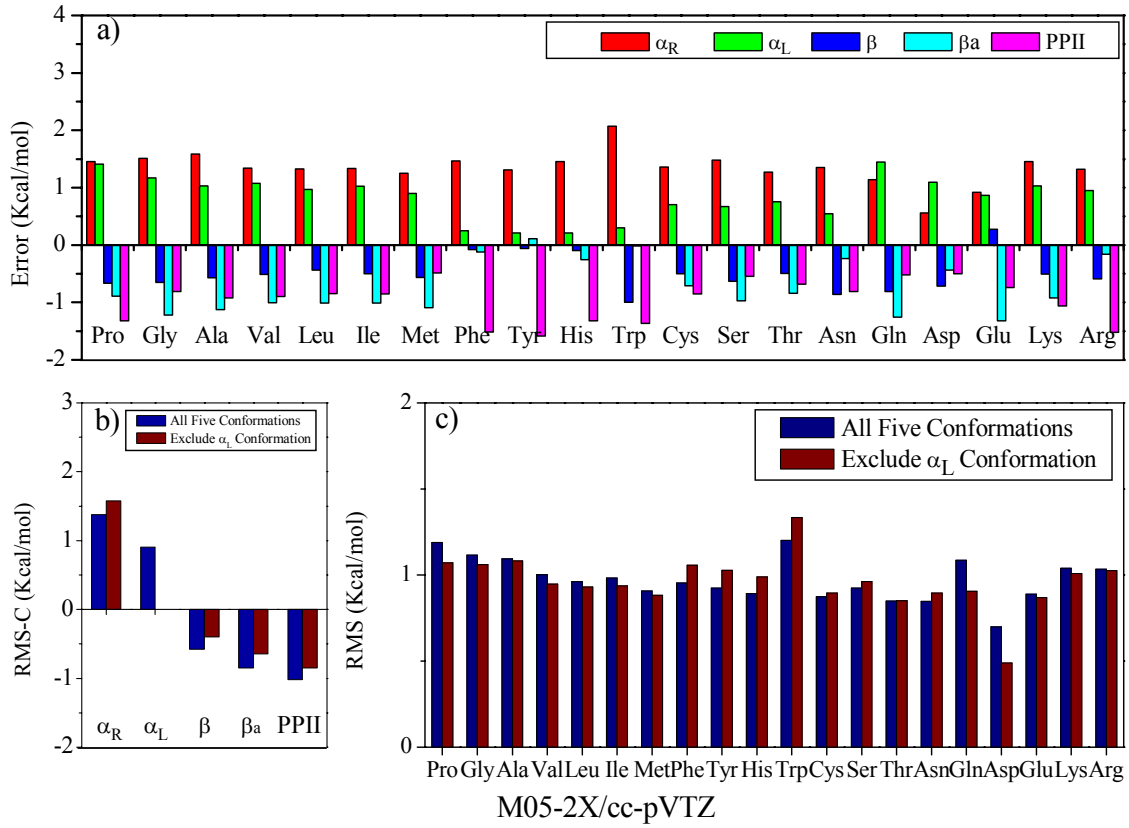

Figure S2. The performance of M05-2X/cc-pVTZ . a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

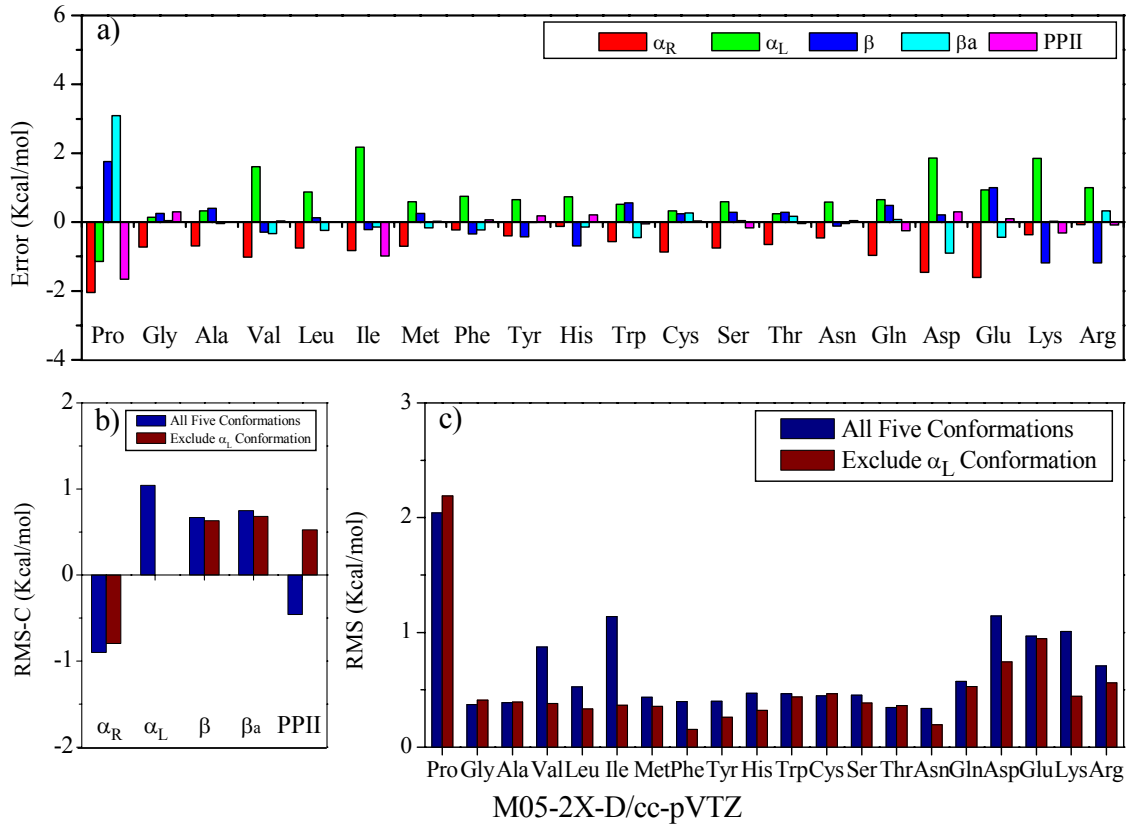

Figure S3. The performance of M05-2X/cc-pVTZ with the AMBER99 dispersion correction. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

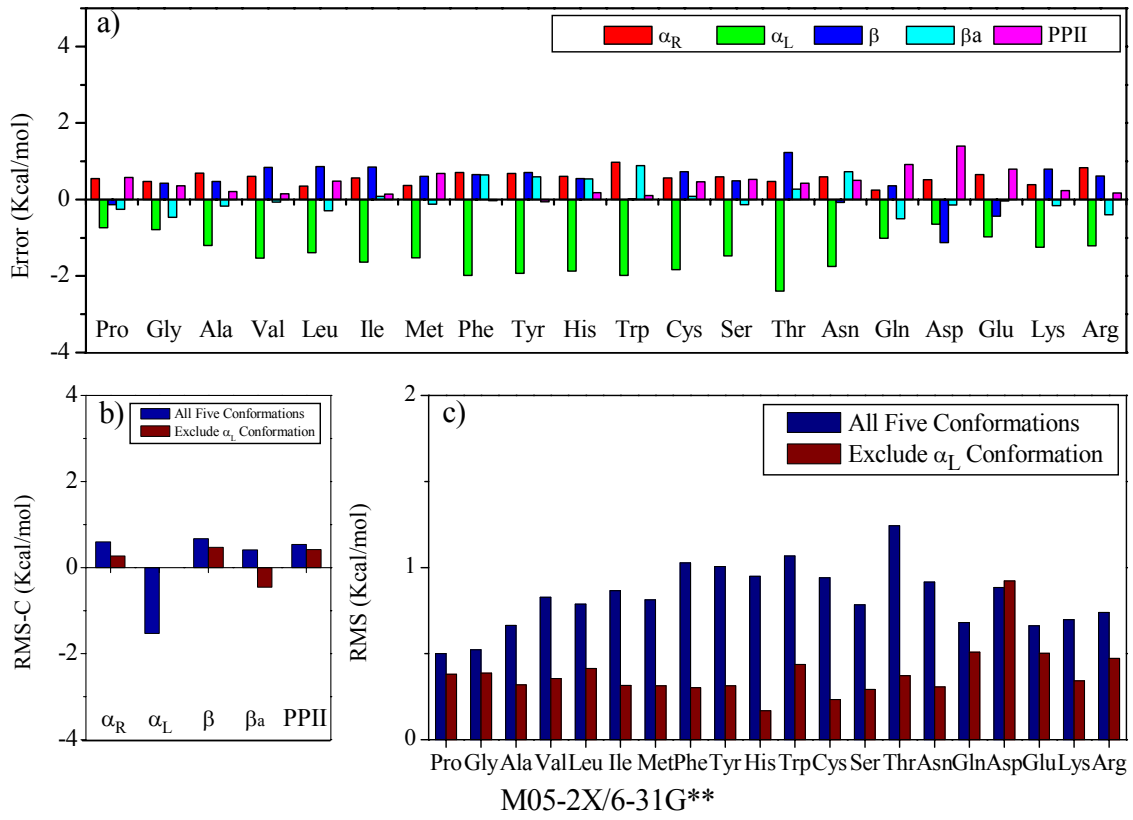

Figure S4. The performance of M05-2X/6-31G**. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

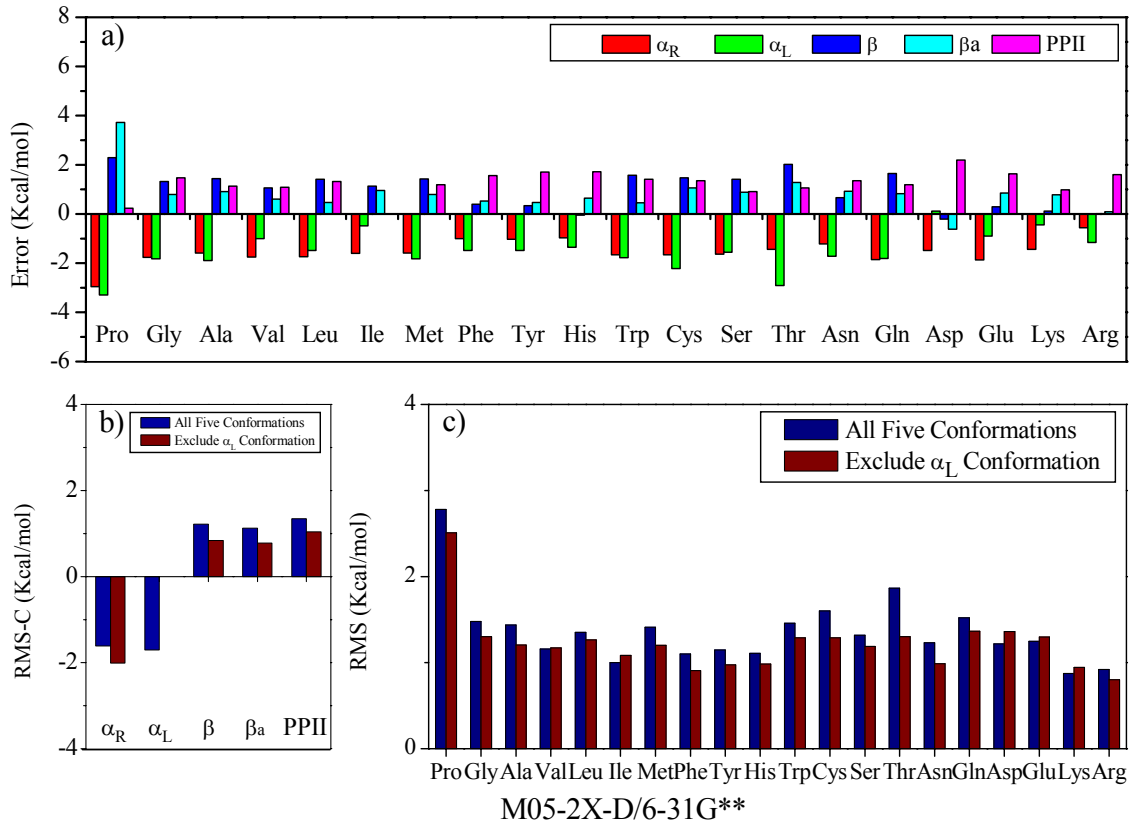

Figure S5. The performance of M05-2X/6-31G** with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

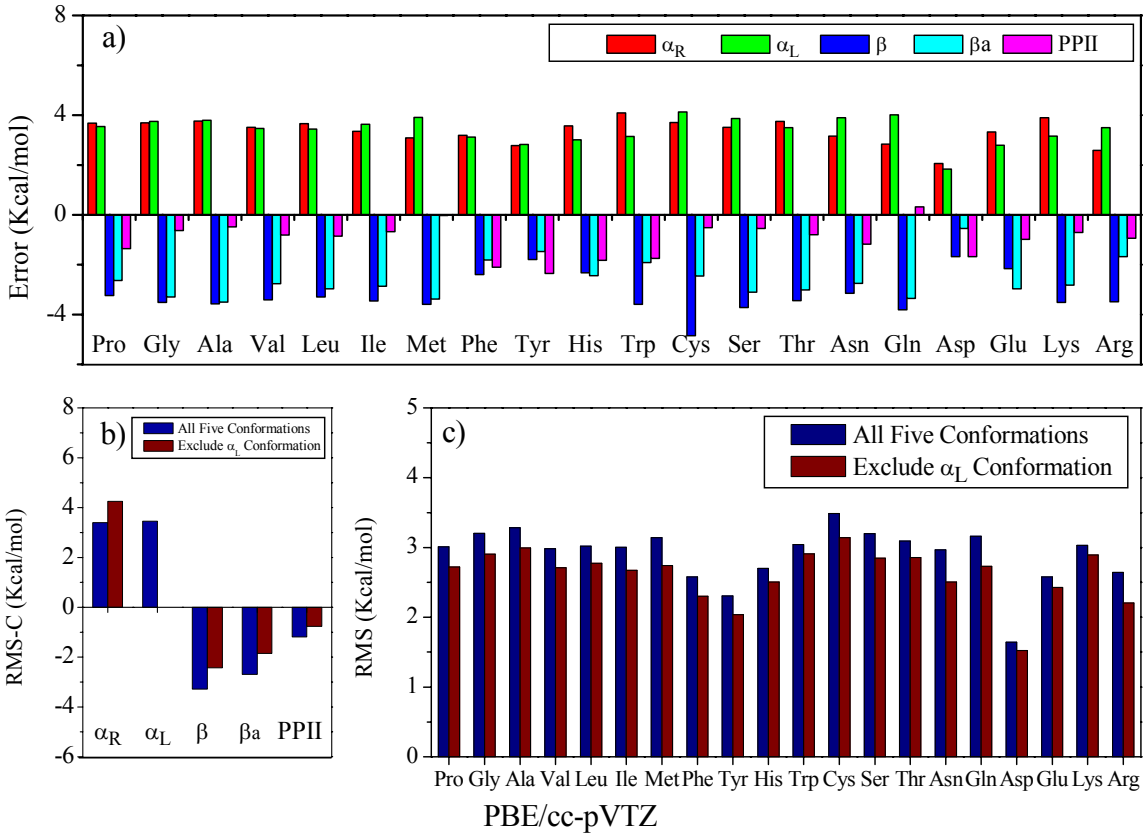

Figure S6. The performance of PBE/cc-pVTZ. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

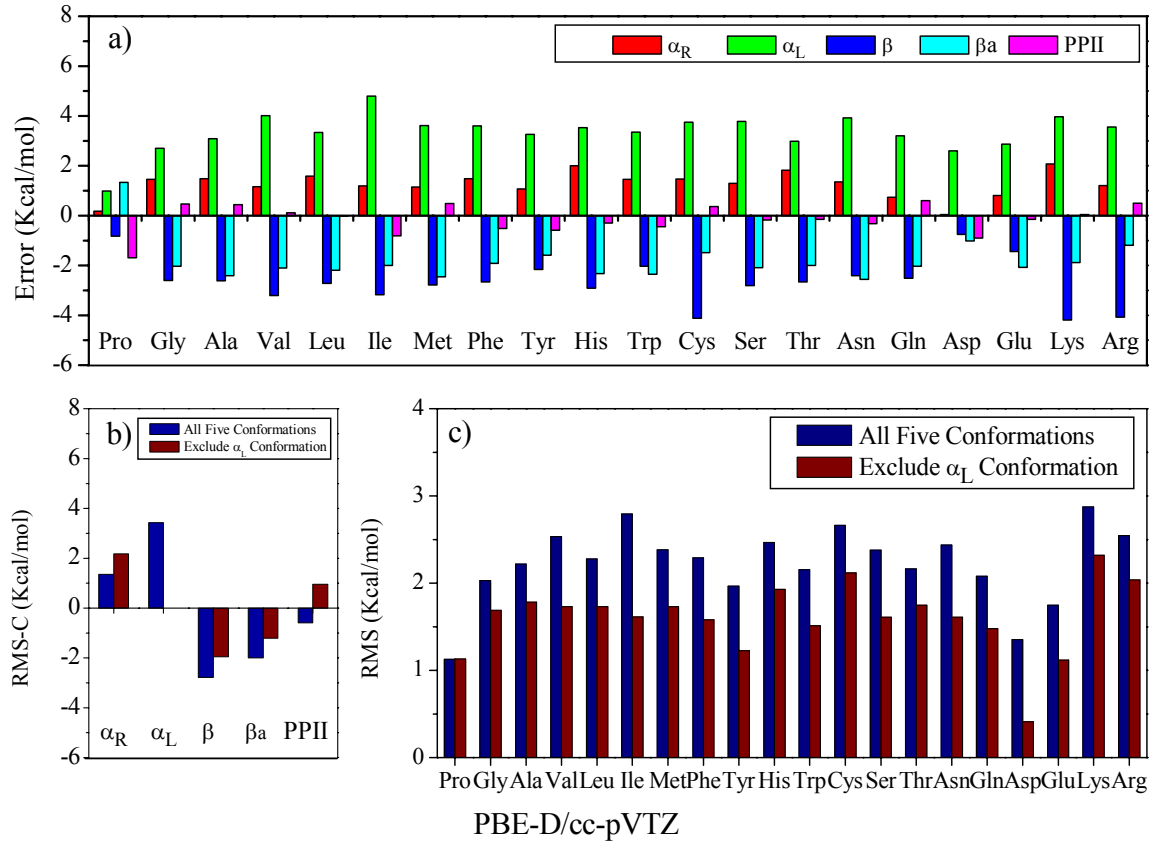

Figure S7. The performance of PBE/cc-pVTZ with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

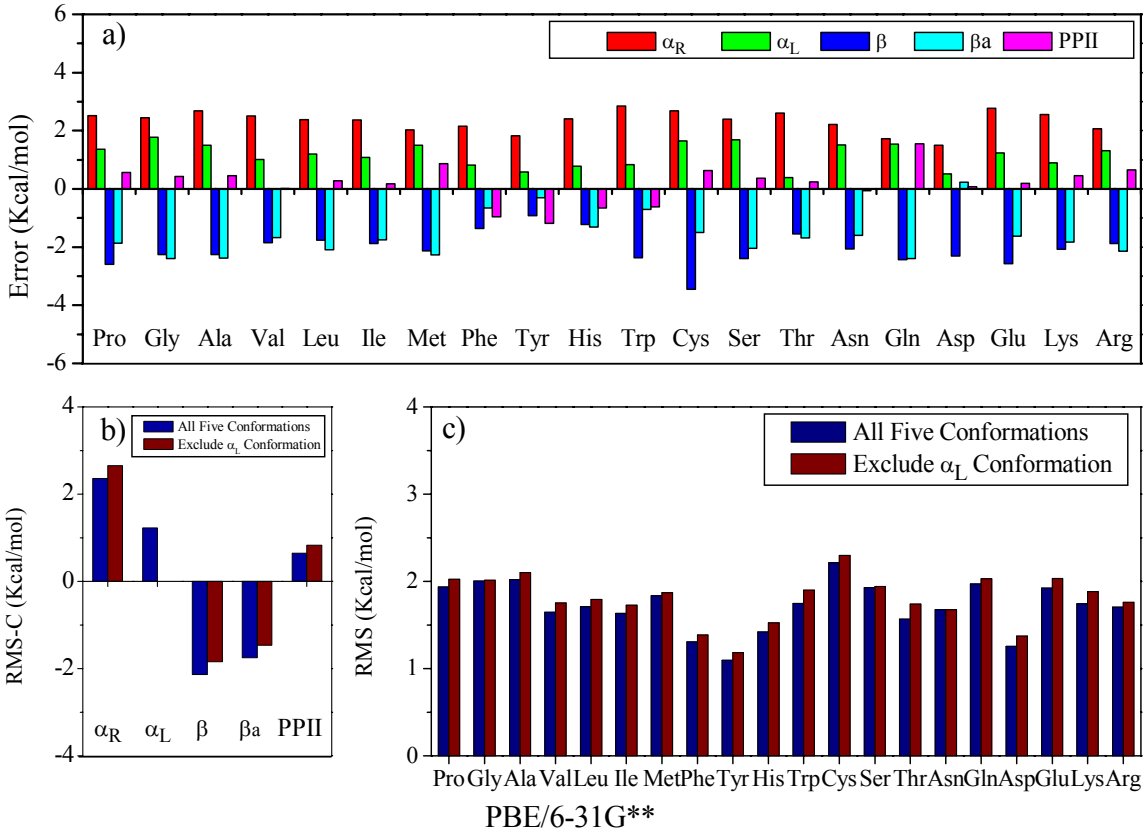

Figure S8. The performance of PBE/6-31G**. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

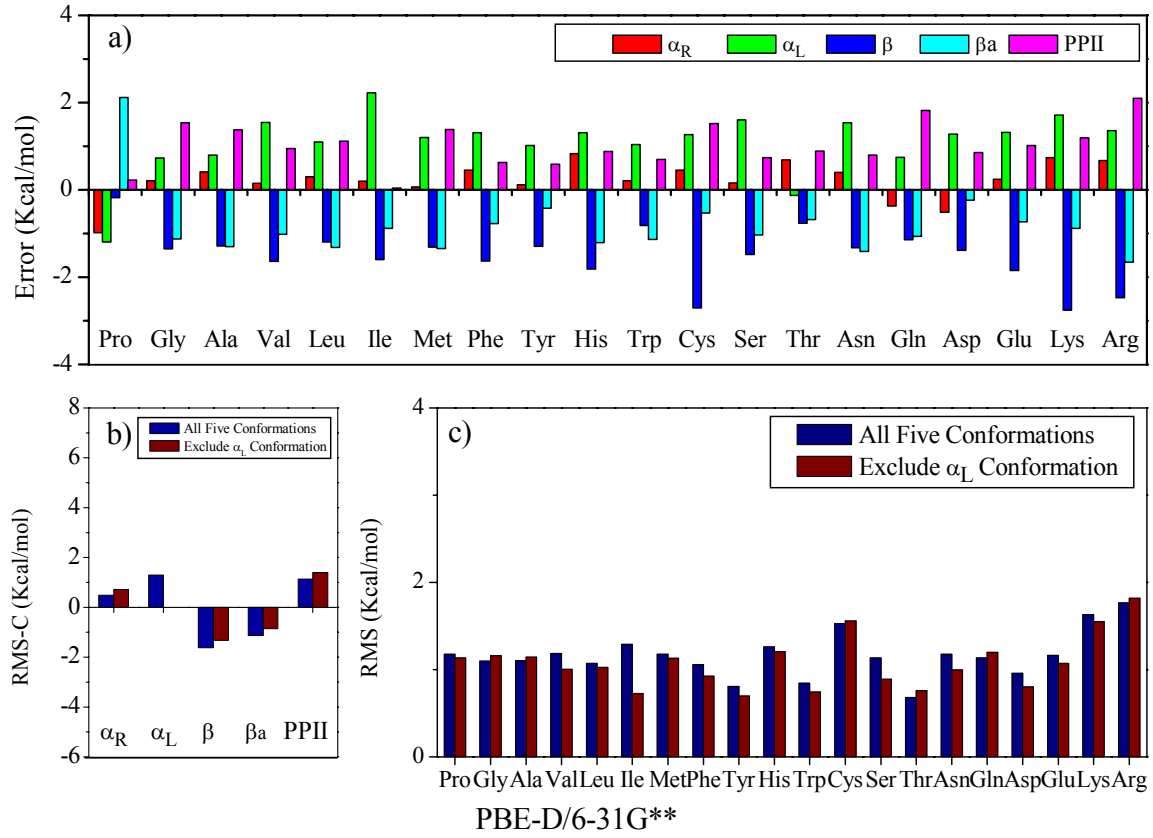

Figure S9. The performance of PBE/6-31G** with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

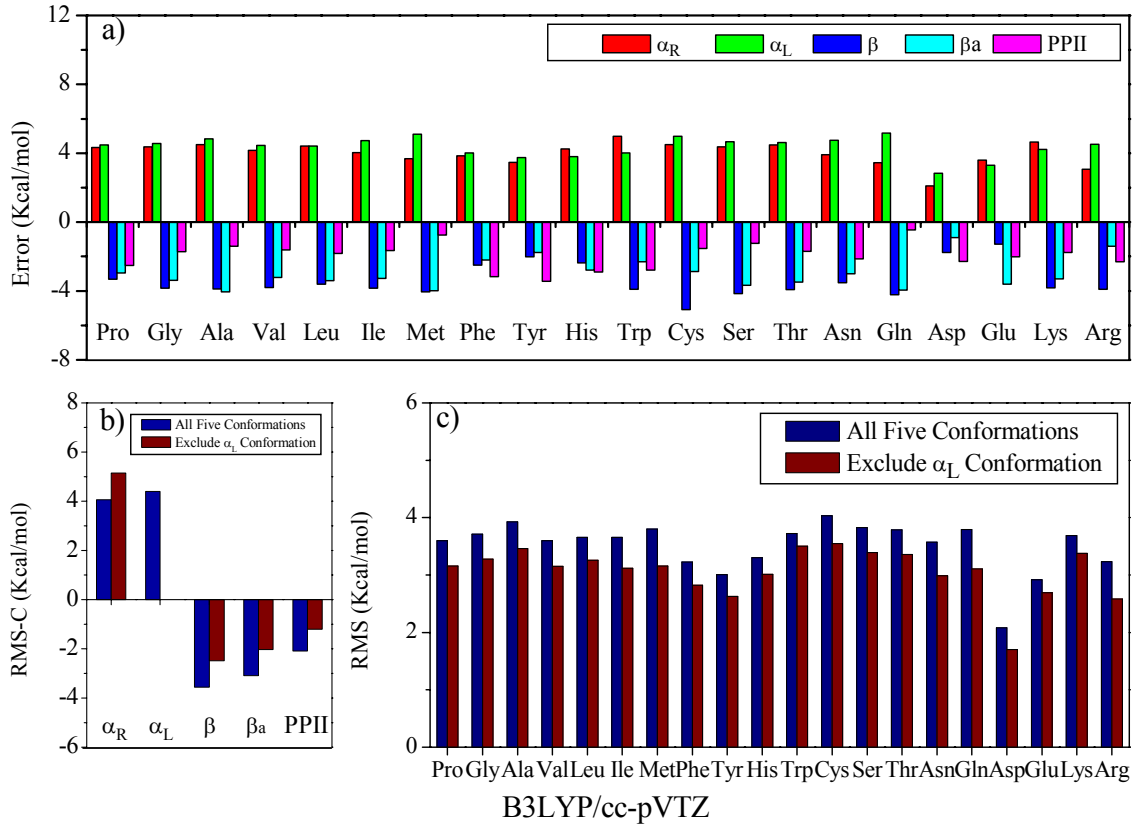

Figure S10. The performance of B3LYP/cc-pVTZ. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

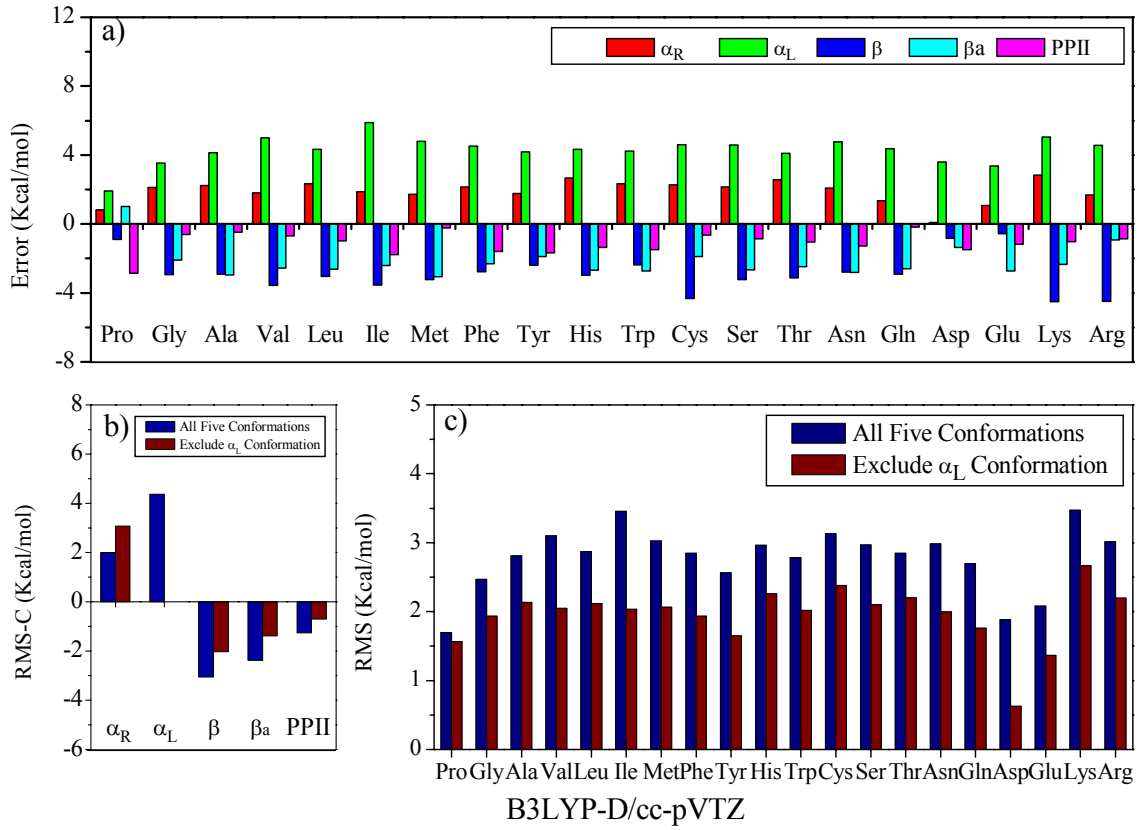

Figure S11. The performance of B3LYP/cc-pVTZ with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

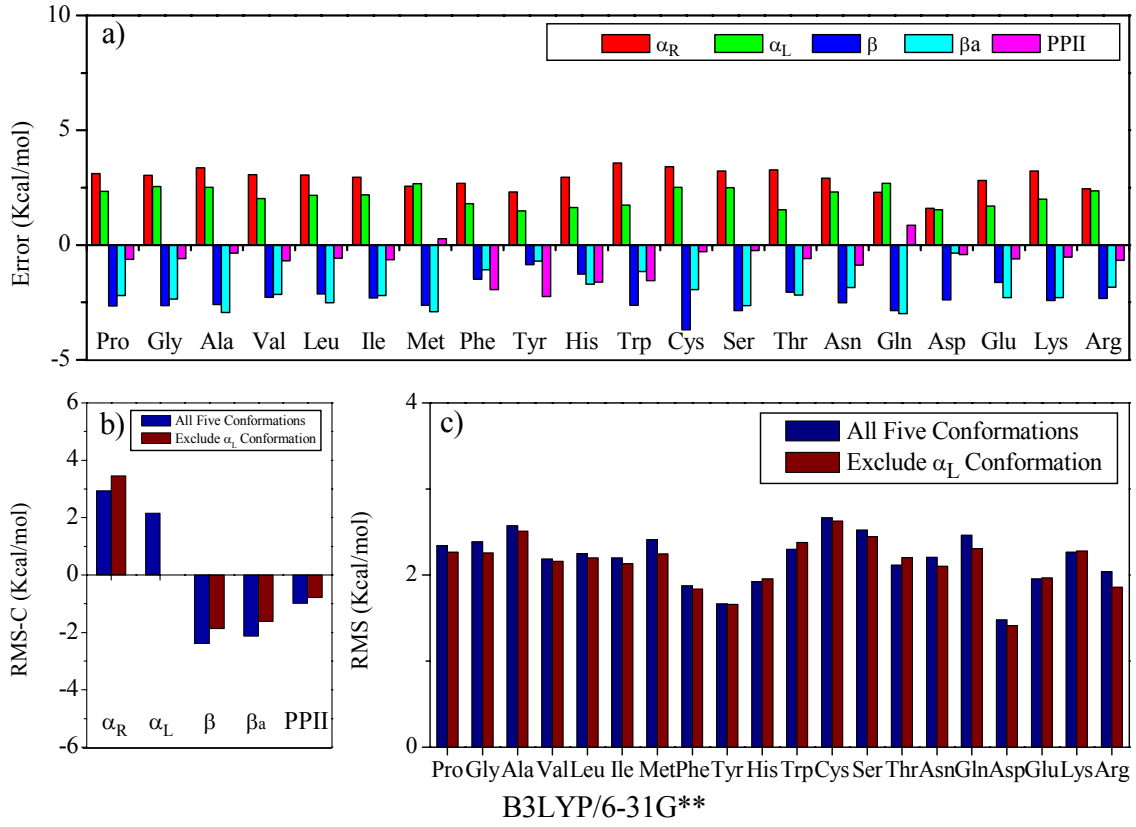

Figure S12. The performance of B3LYP/6-31G**. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

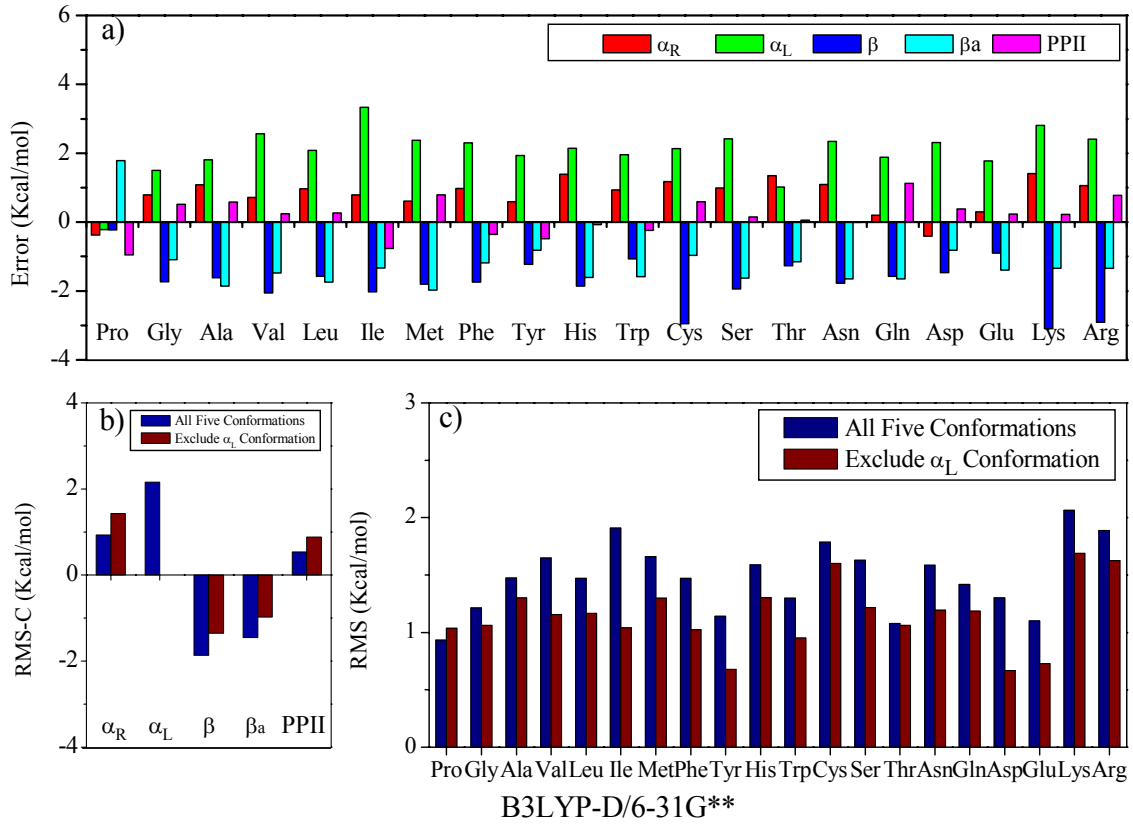

Figure S13. The performance of B3LYP/6-31G** with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

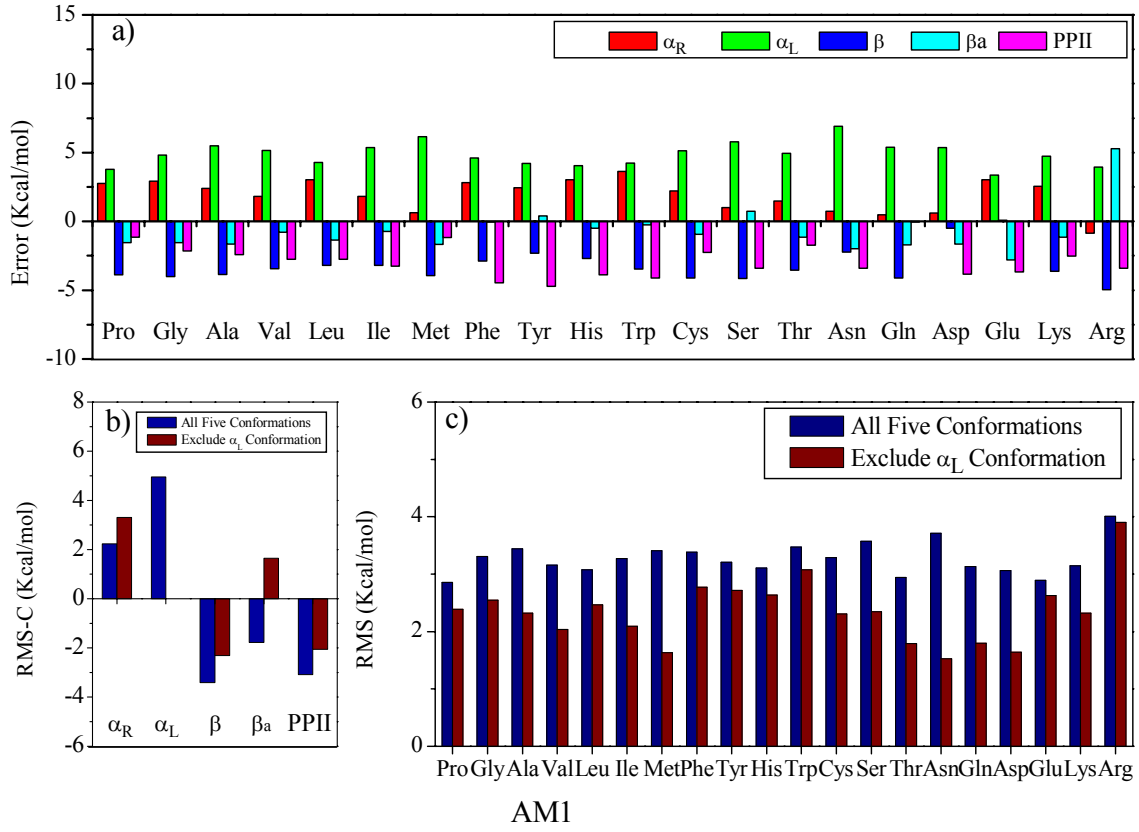

Figure S14. The performance of AM1. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

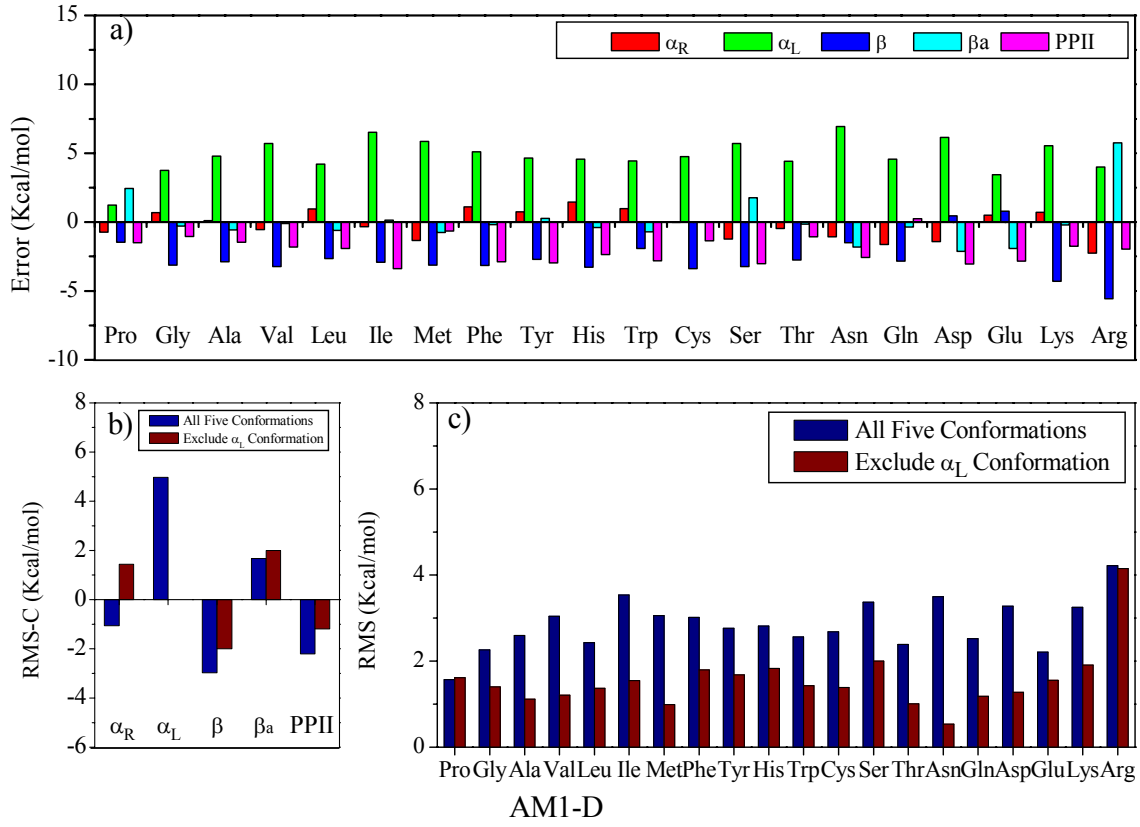

Figure S15. The performance of AM1 with AMBER99 dispersion energy. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

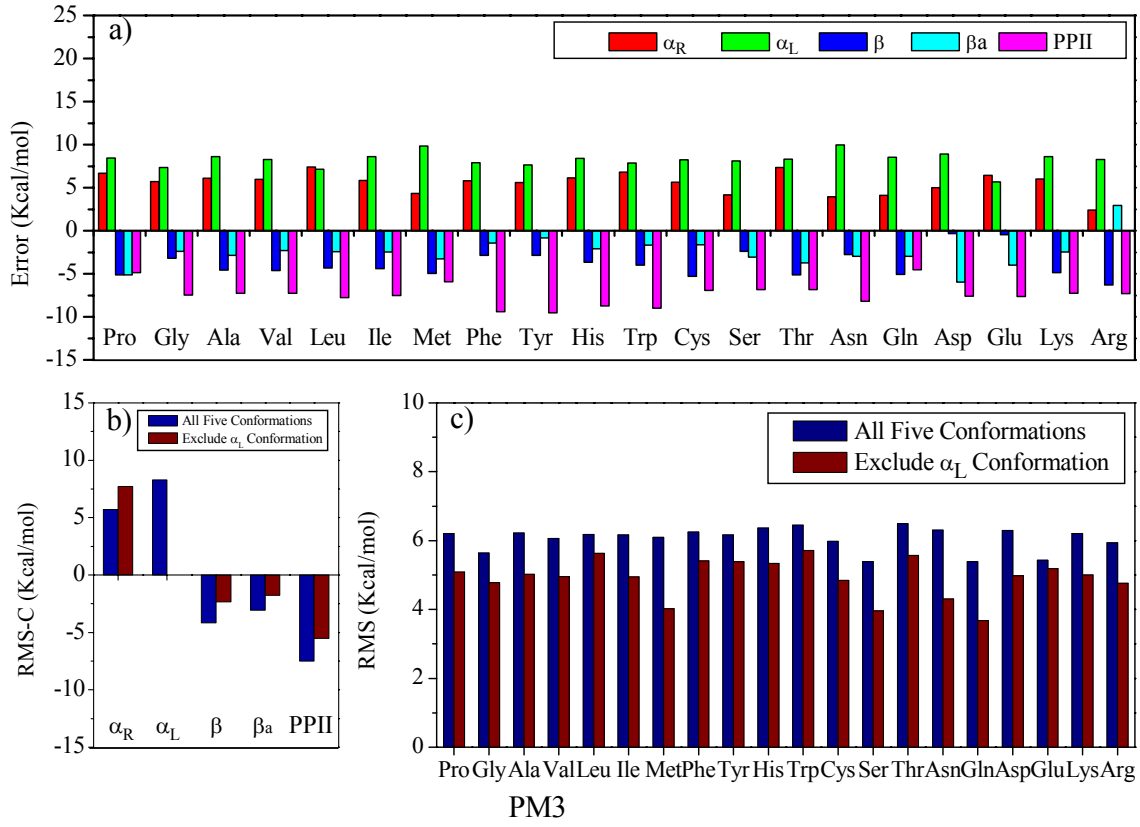

Figure S16. The performance of PM3. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

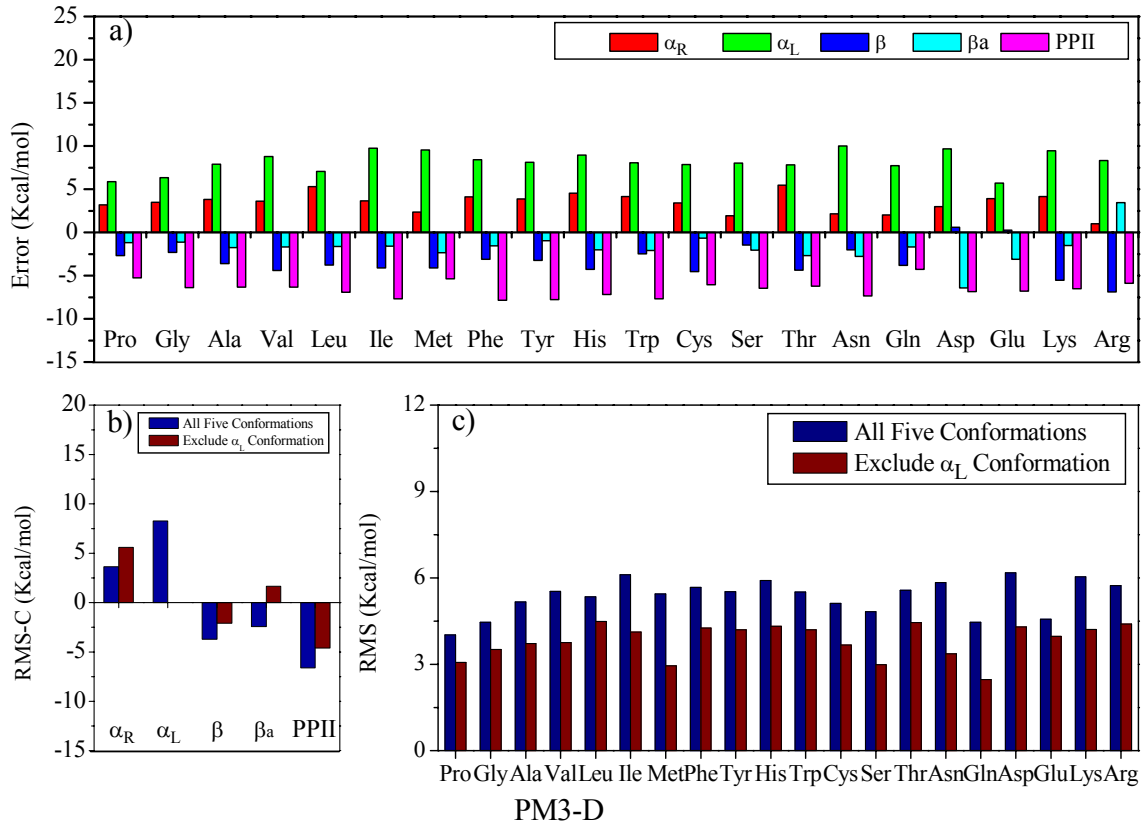

Figure S17. The performance of PM3 with AMBER99 dispersion energy. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

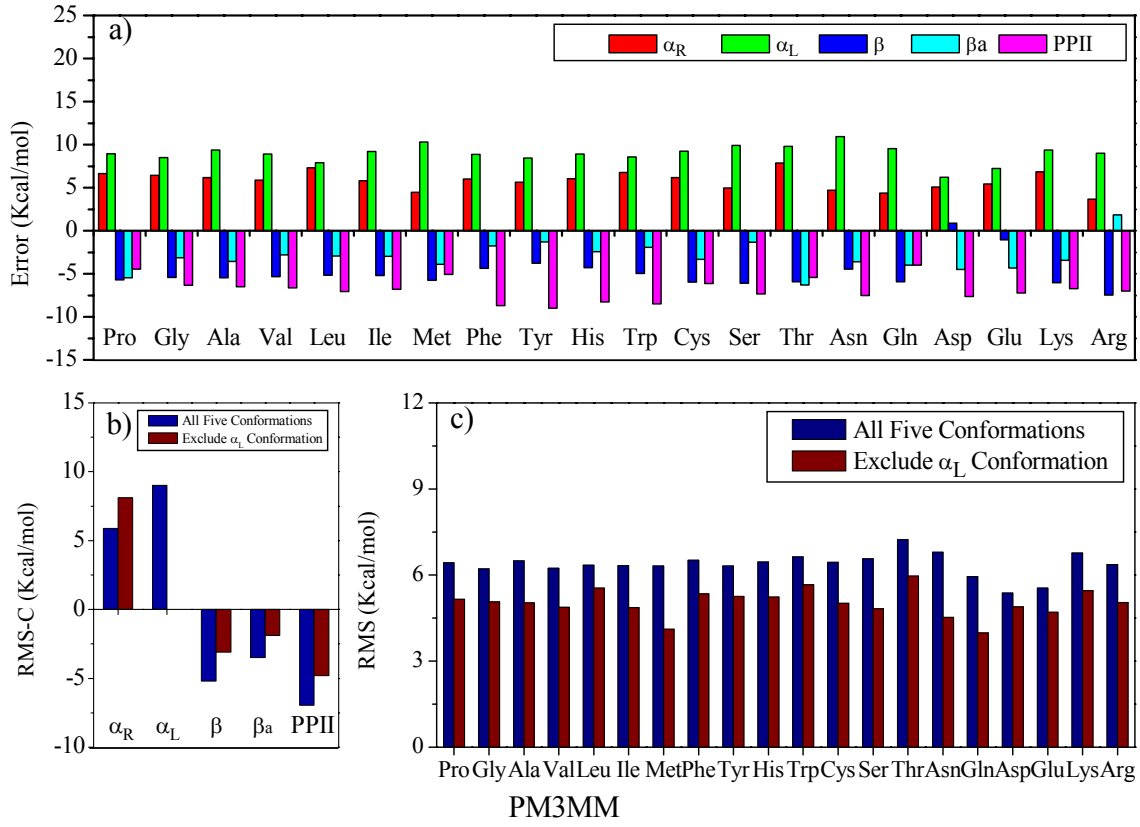

Figure S18. The performance of PM3MM. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

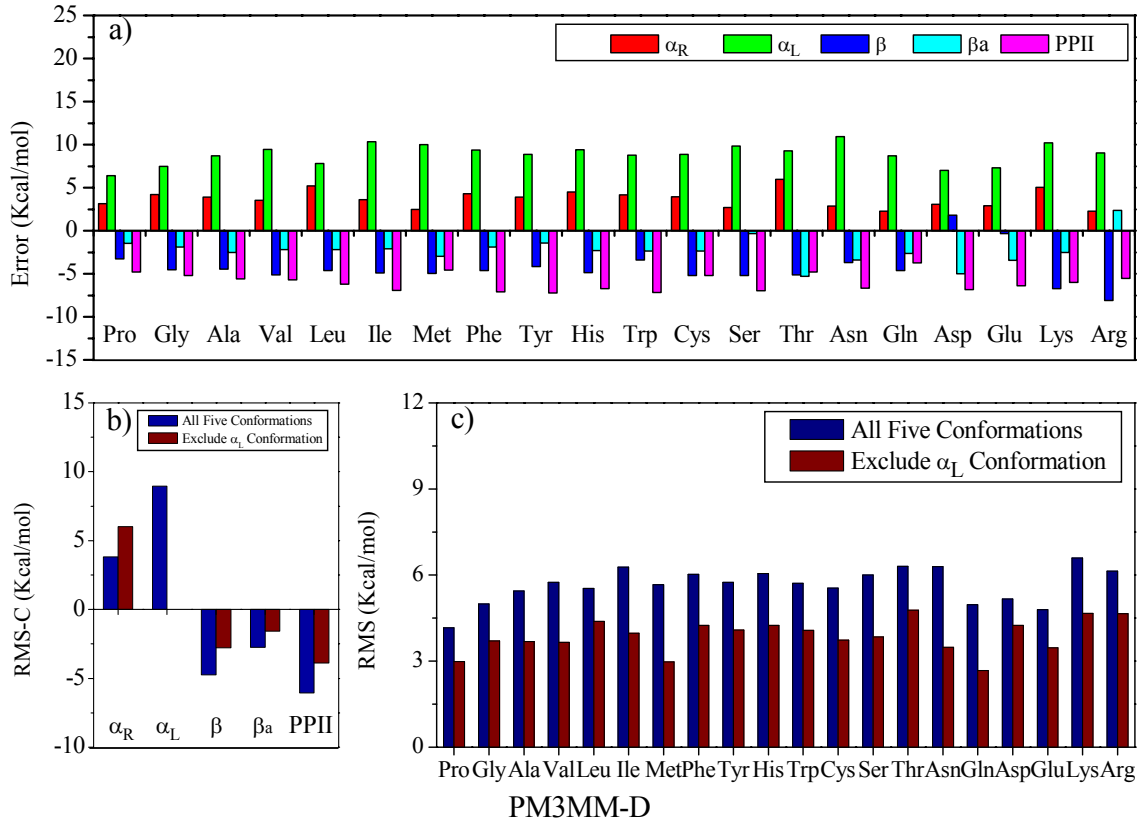

Figure S19. The performance of PM3MM with AMBER99 dispersion energy. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

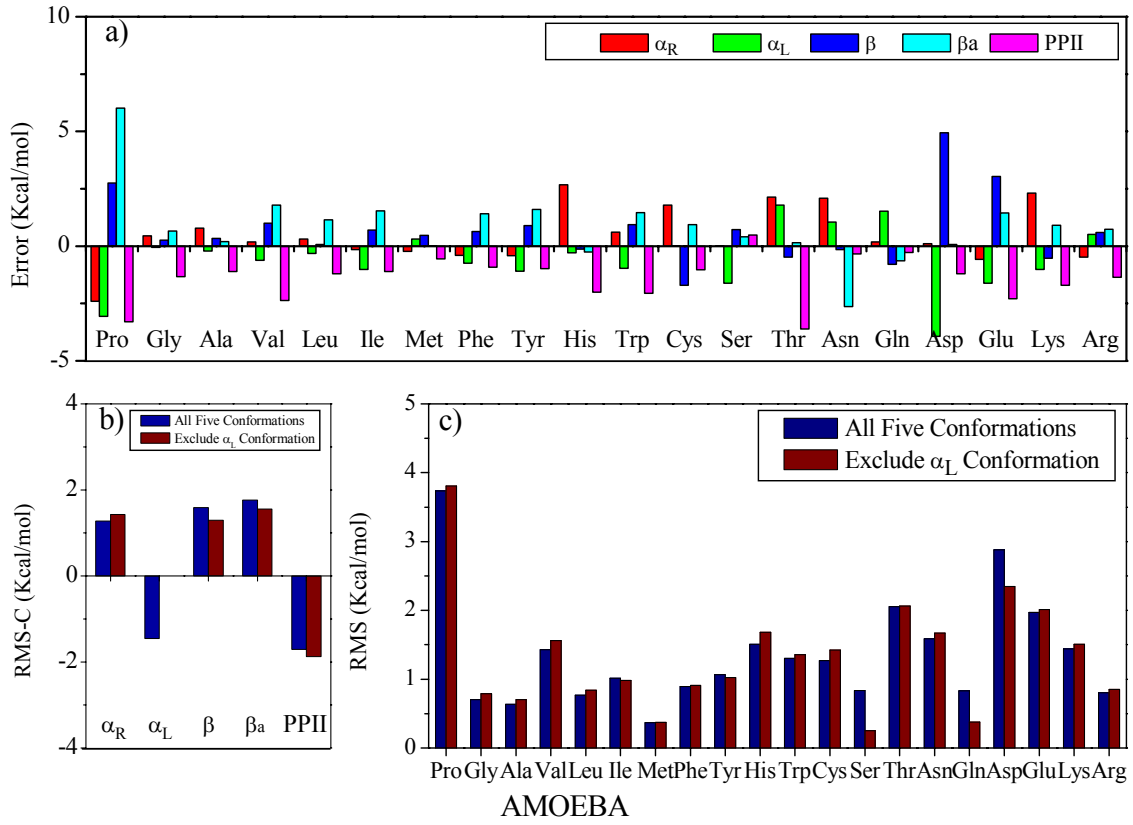

Figure S20. The performance of force field AMOEBA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

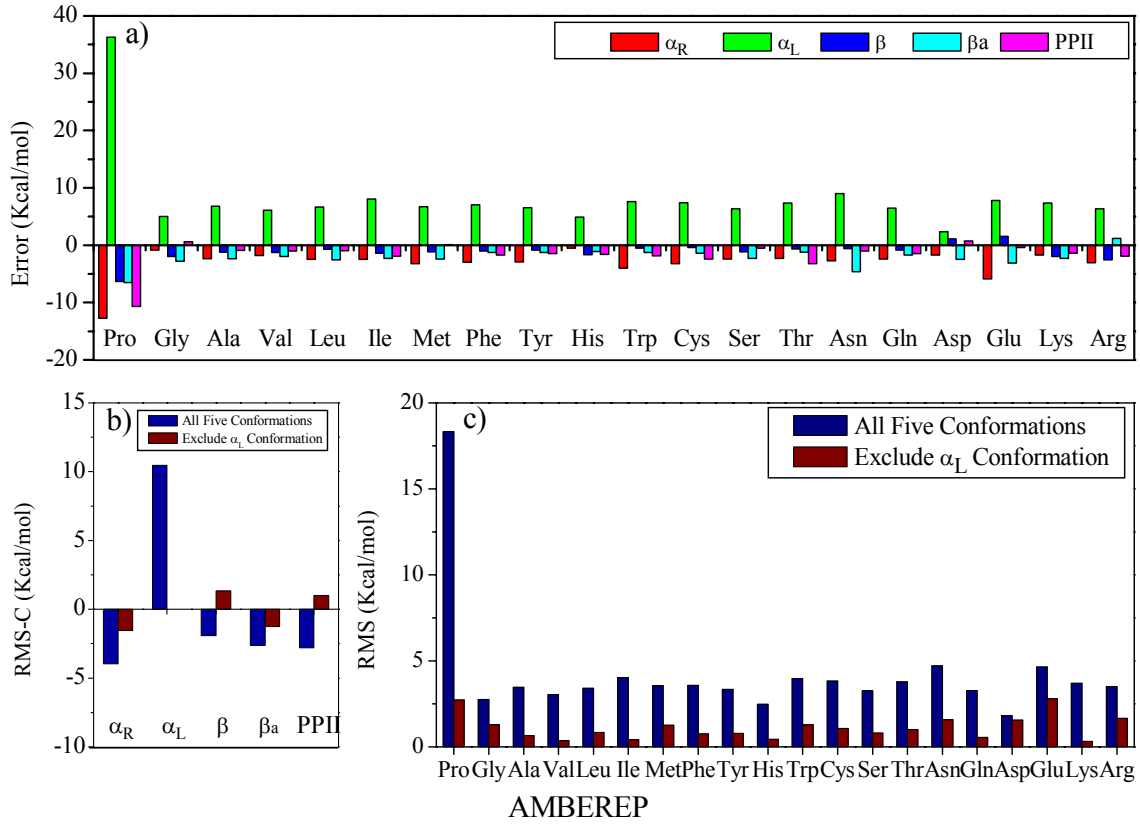

Figure S21. The performance of force field AMBEREP. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

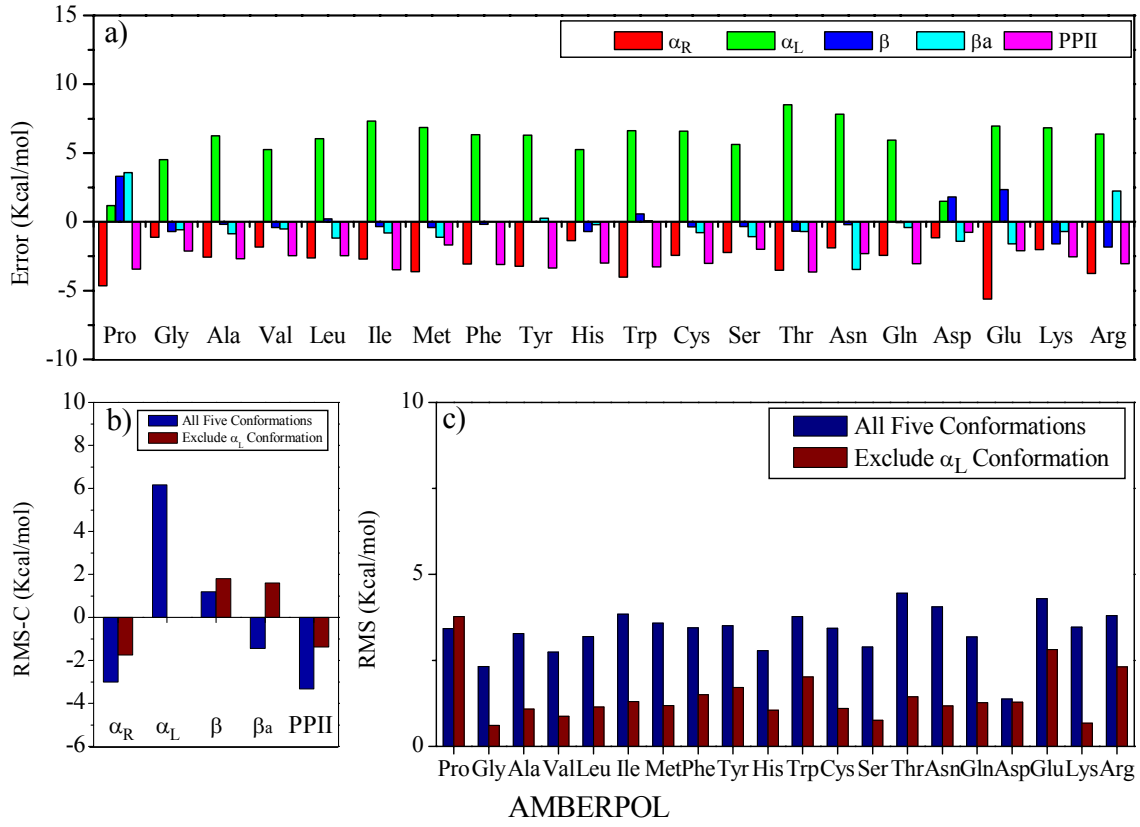

Figure S22. The performance of force field AMBERPOL. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

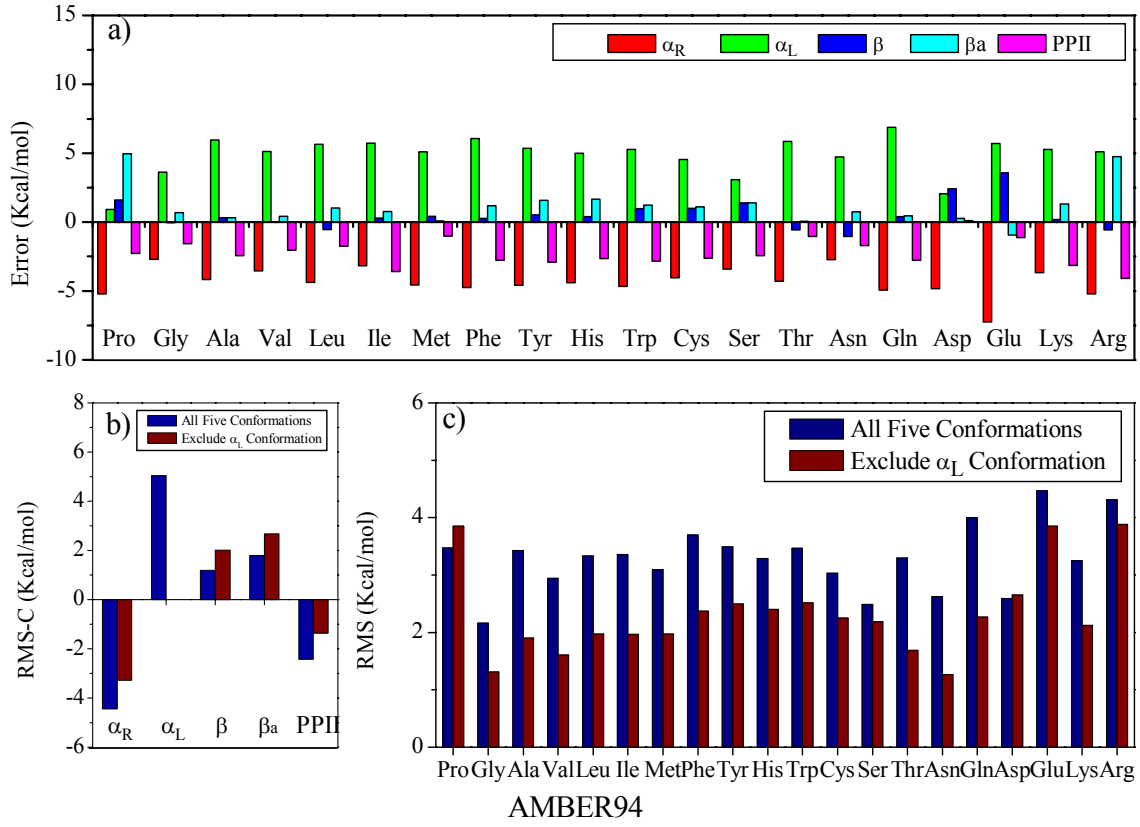

Figure S23. The performance of force field AMBER94. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

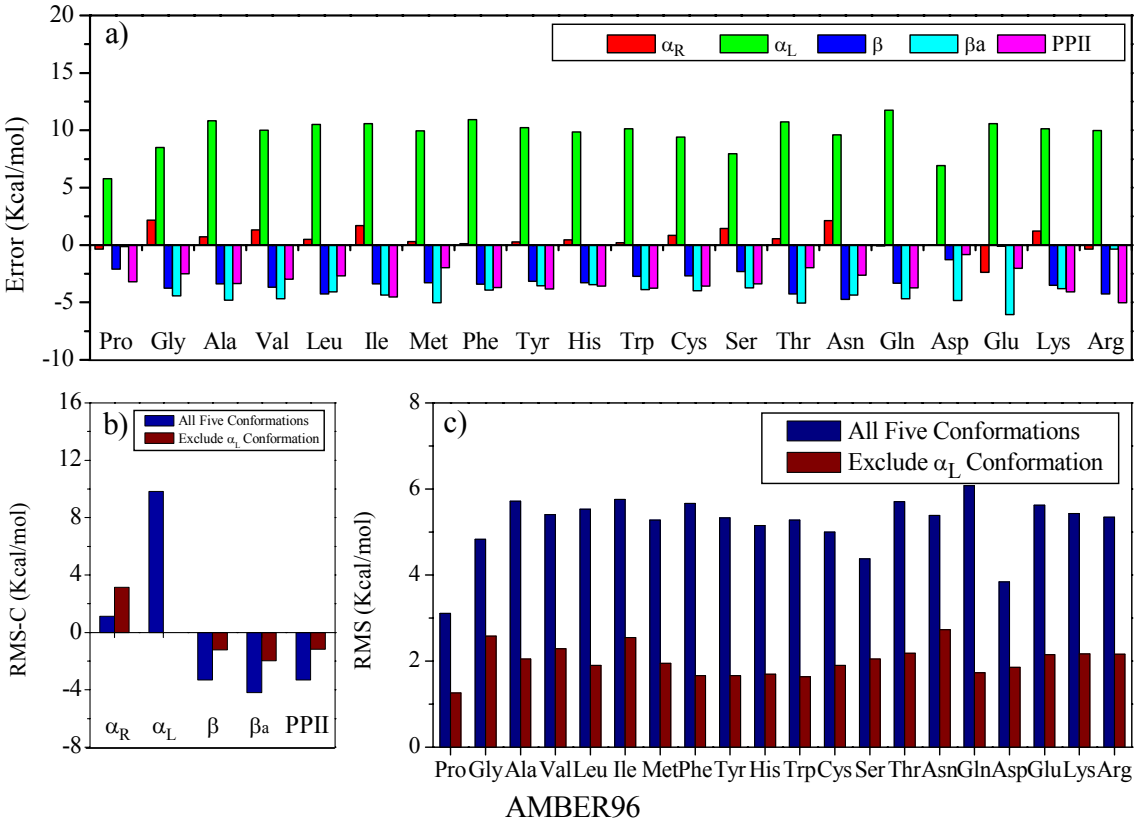

Figure S24. The performance of force field AMBER96. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

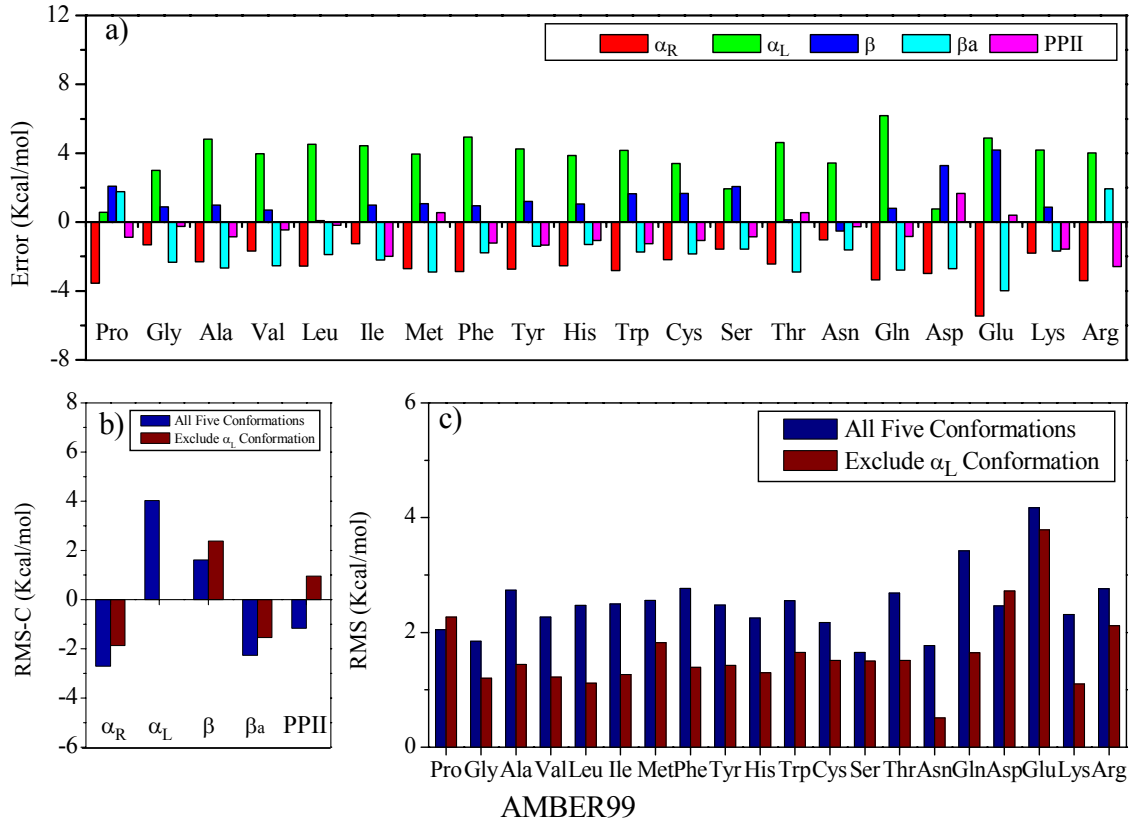

Figure S25. The performance of force field AMBER99. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

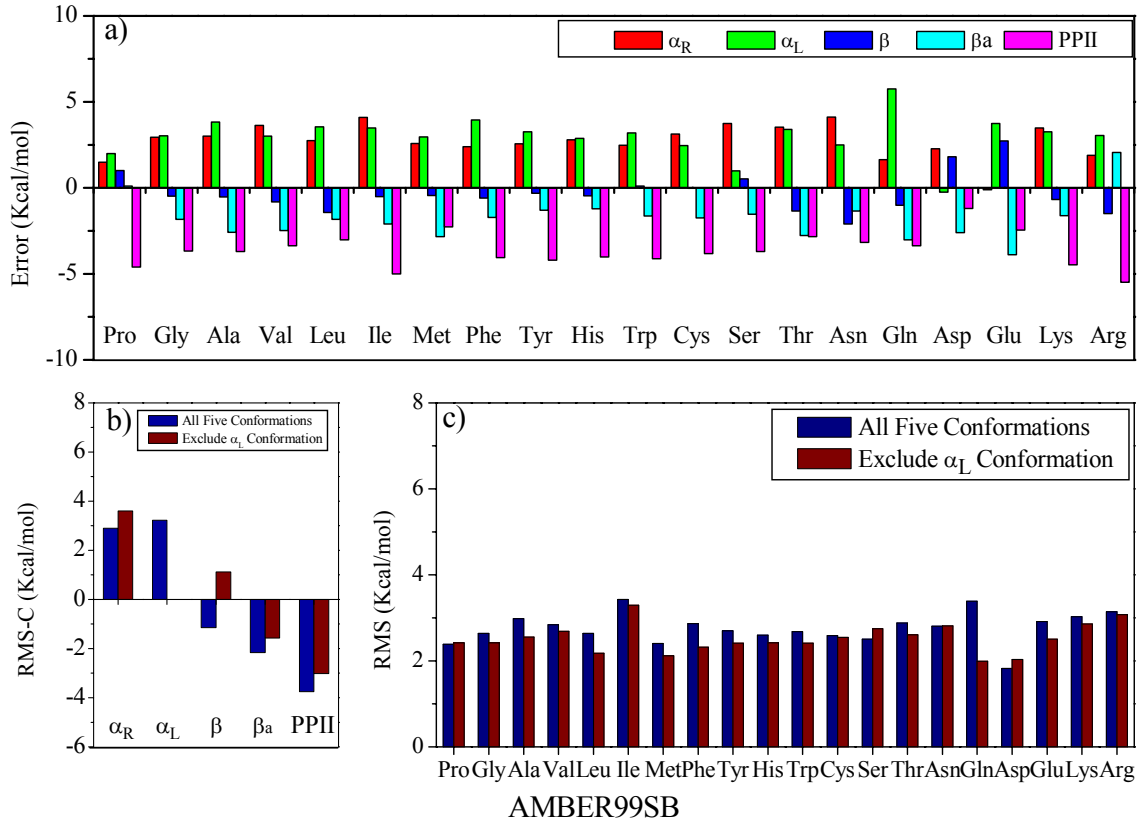

Figure S26. The performance of force field AMBER99SB. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

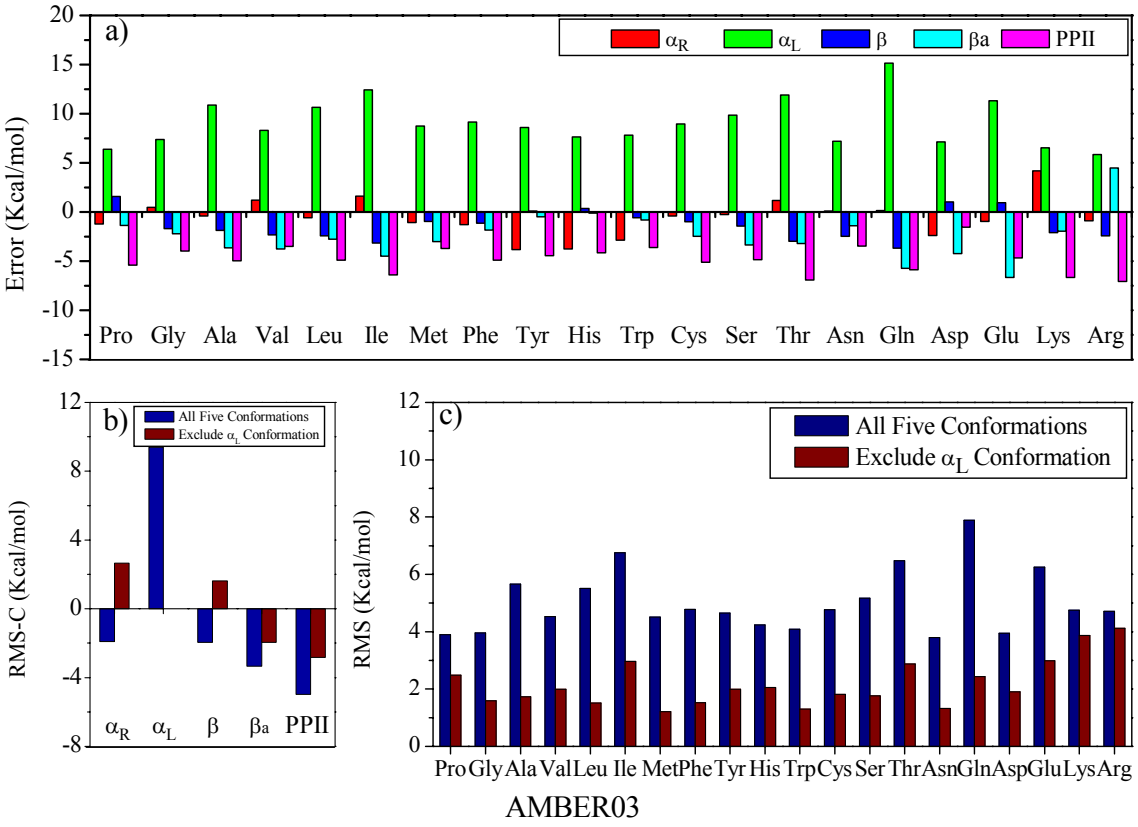

Figure S27. The performance of force field AMBER03. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

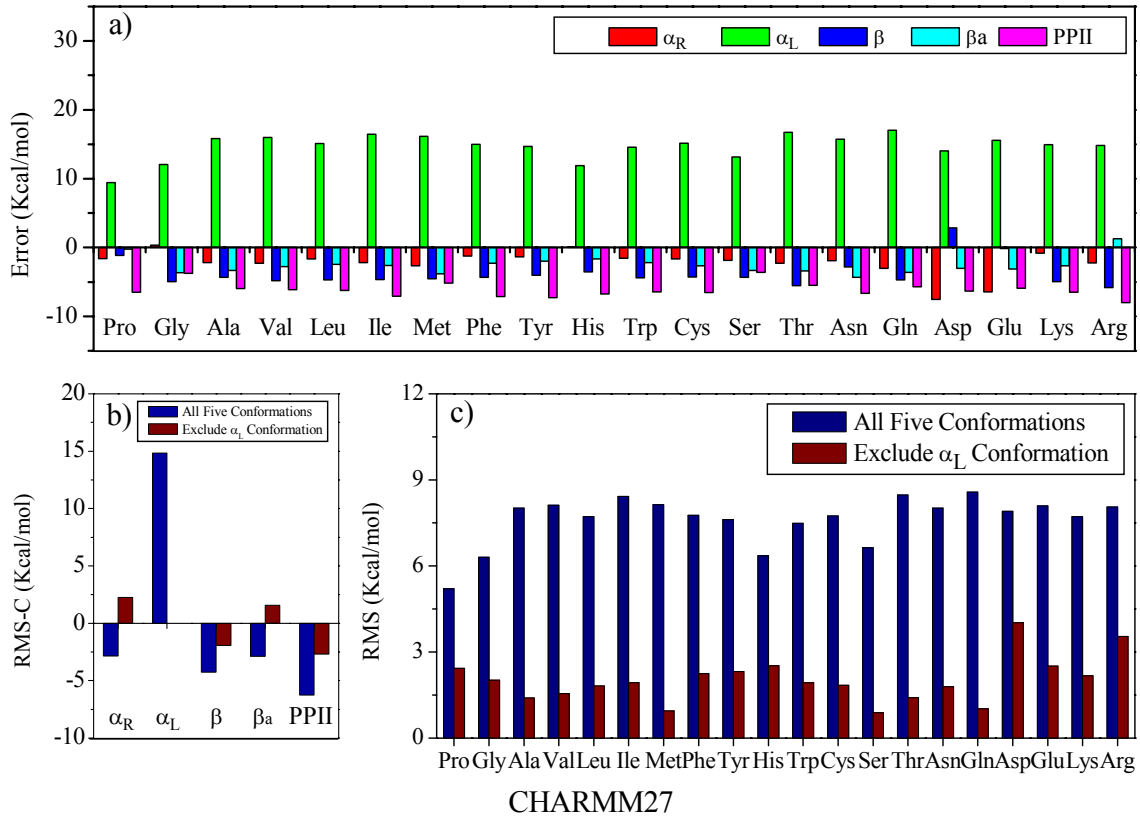

Figure S28. The performance of force field CHARMM27. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

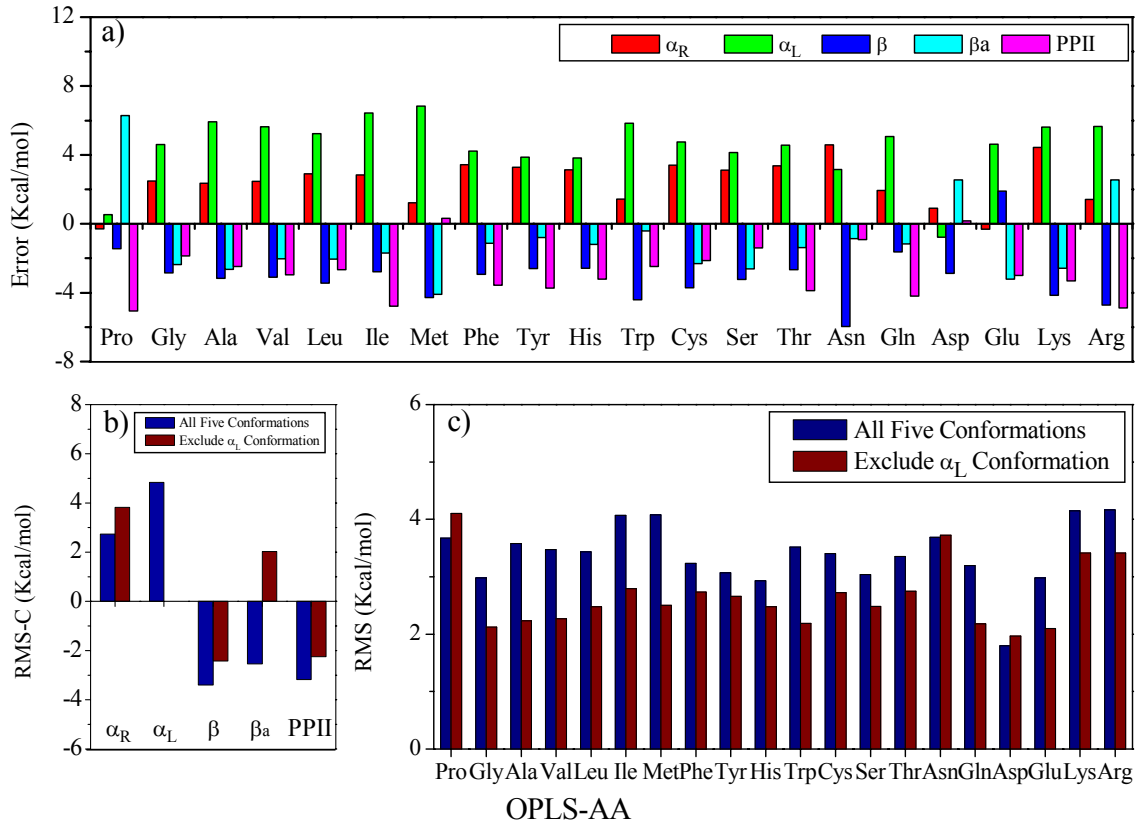

Figure S29. The performance of force field OPLS-AA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

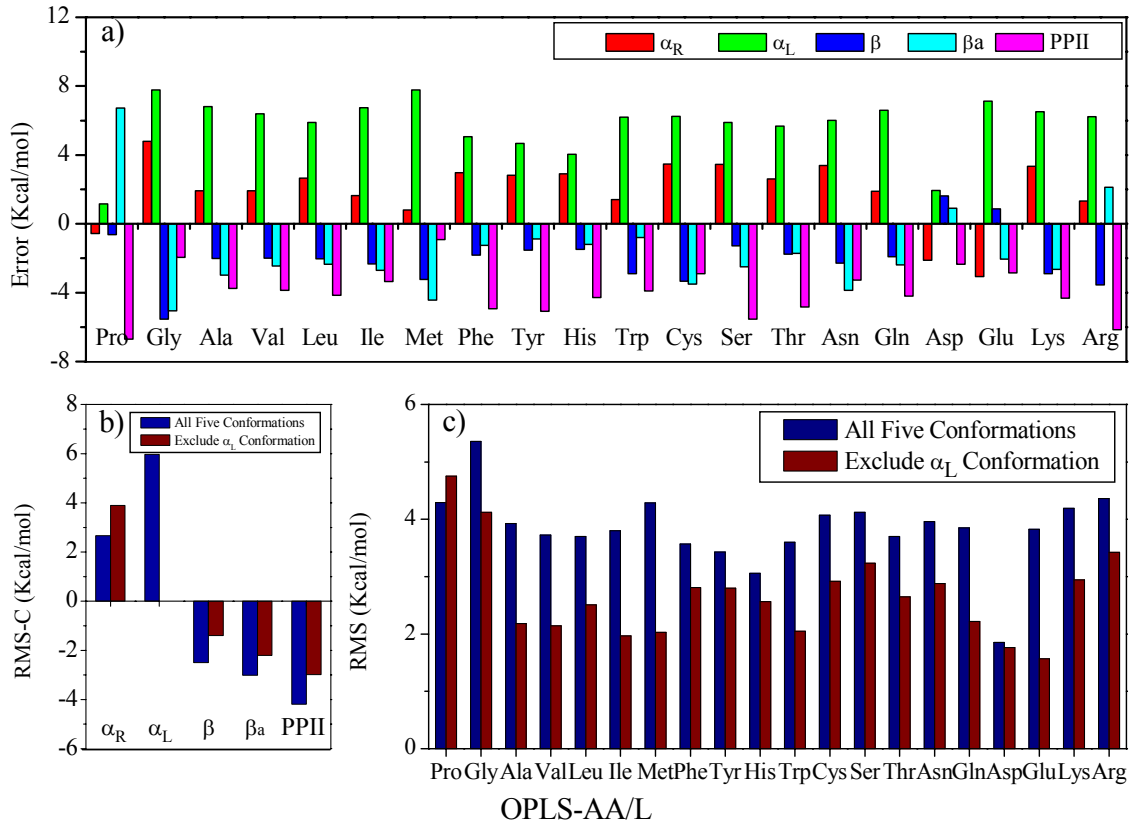

Figure S30. The performance of force field OPLS-AA/L. a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

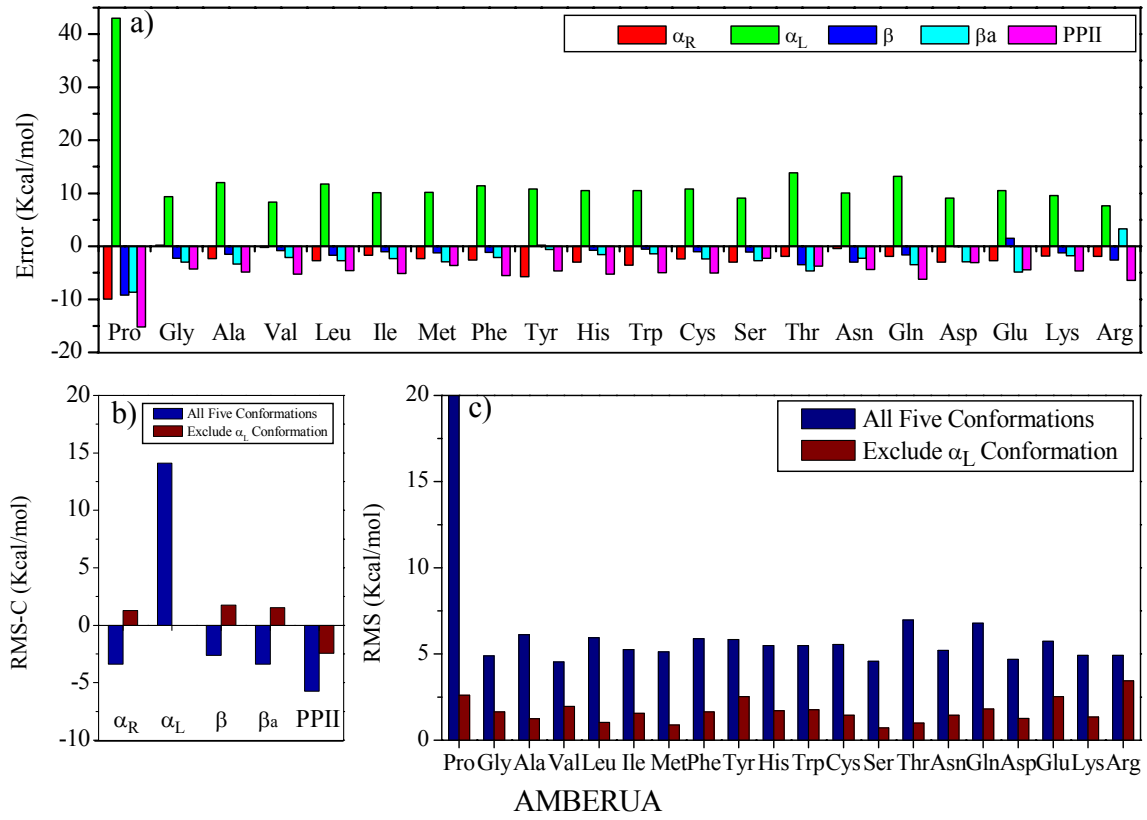

Figure S31. The performance of force field AMBERUA. a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

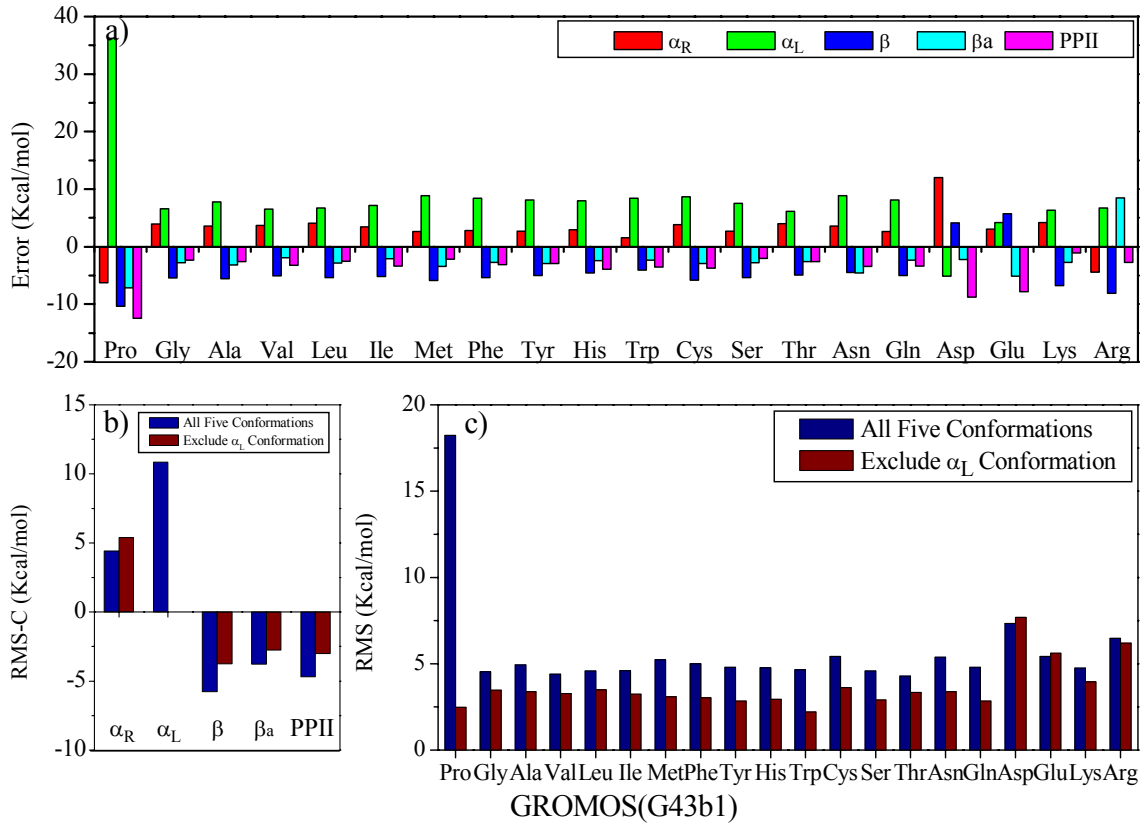

Figure S32. The performance of force field GROMOS(G43b1). a) Signed error (*error*=E_{ai}-E_{bi}+E_c) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

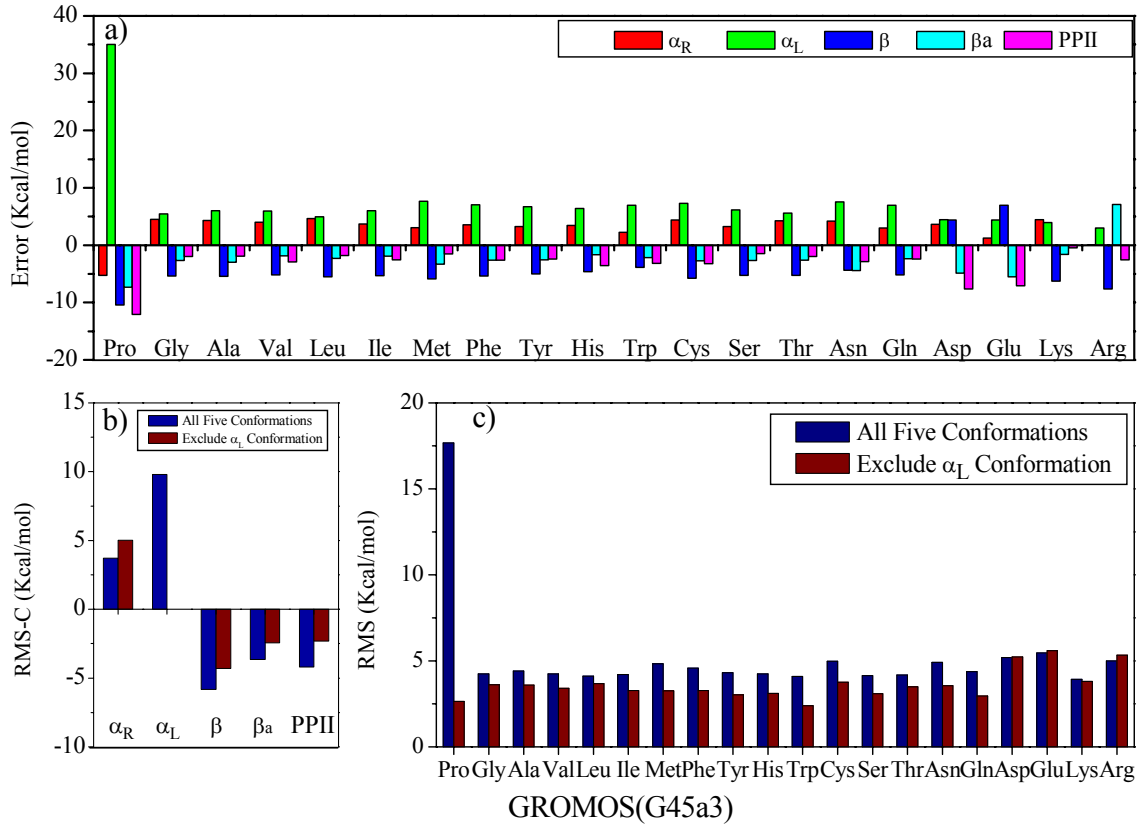

Figure S33. The performance of force field GROMOS(G45a3). a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

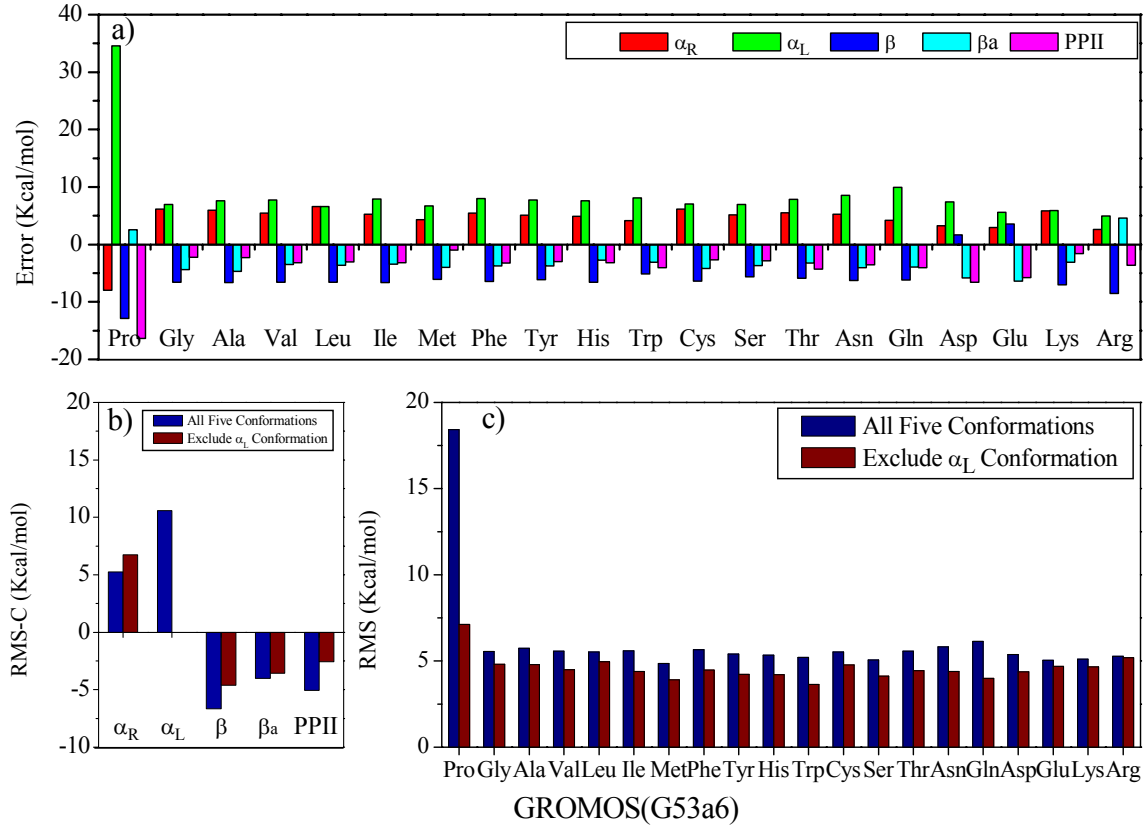

Figure S34. The performance of force field GROMOS(G53a6). a) Signed error ($error=E_{ai}-E_{bi}+E_c$) using the MP2 energy as the true value. b) Signed RMS-C of each conformation over 20 amino acids. c) RMS over the five conformations of each amino acid.

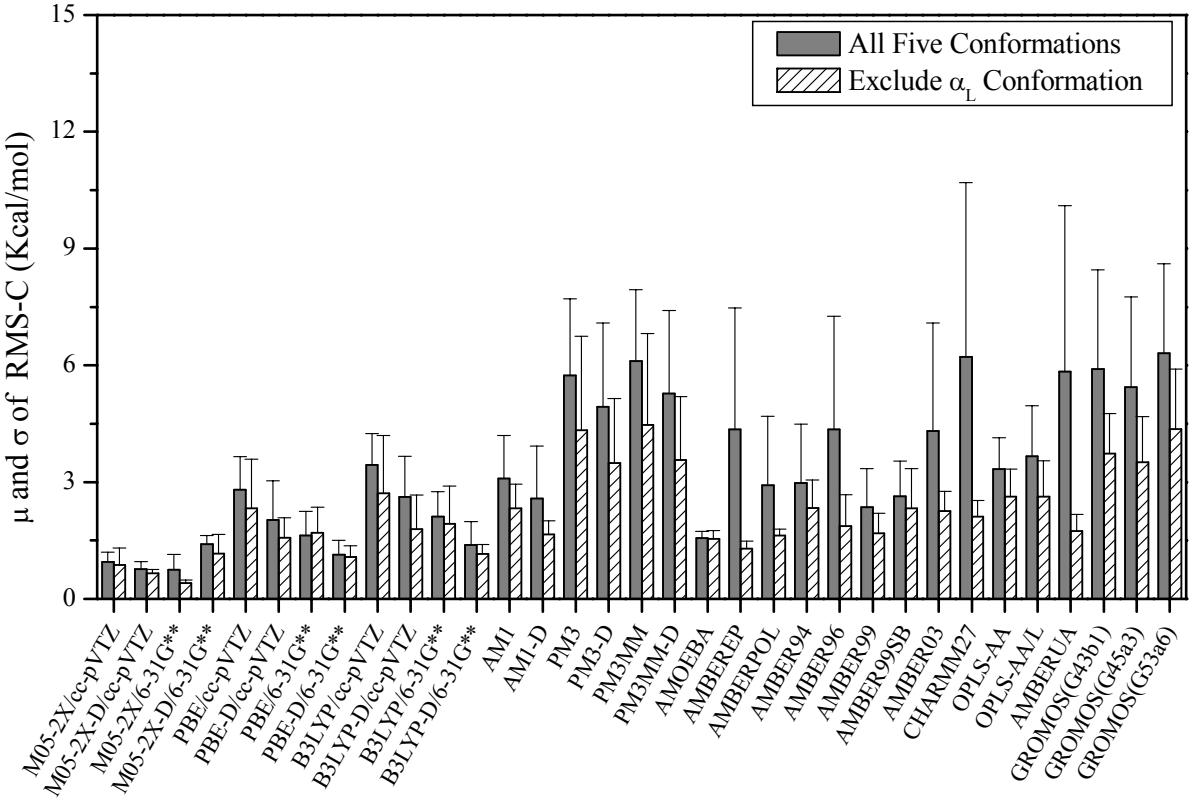

Figure S35. Mean and stand deviation of RMS-C of each conformation calculated over 20 amino acids for each method.

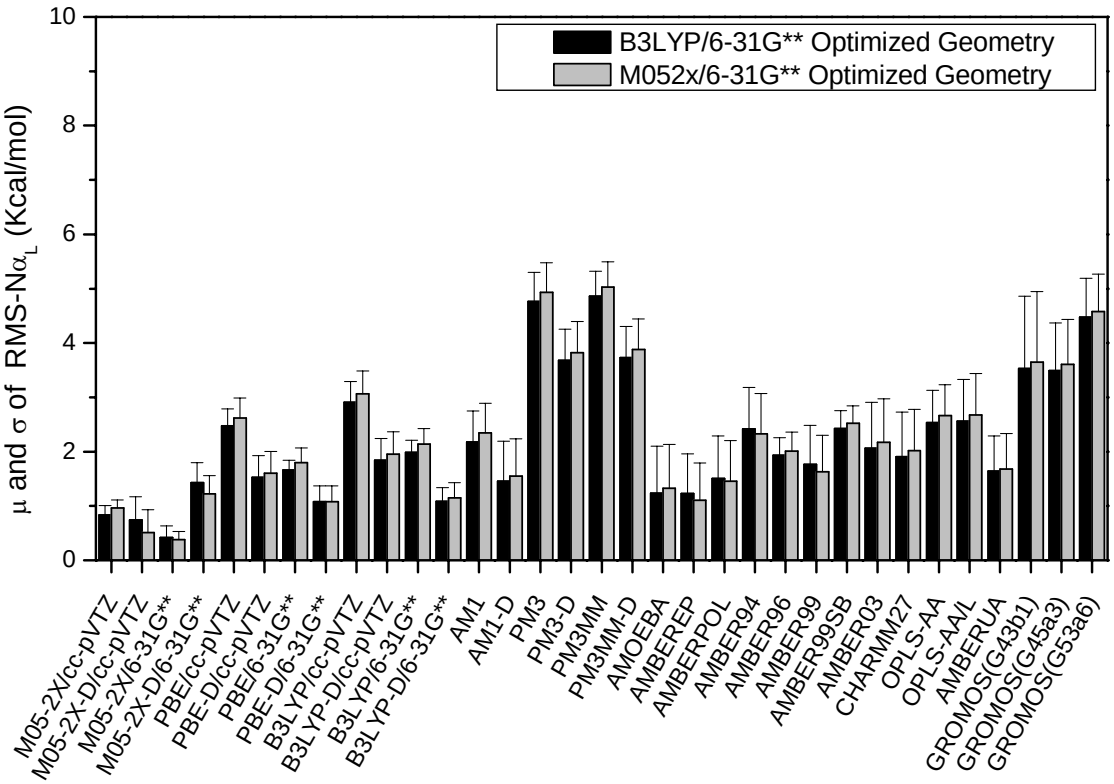

Figure S36. Comparison of the RMS-Nα_L using two set of geometries obtained from two DFT methods (B3LYP/6-31G** and M05-2X/6-31G**).