Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Extensive Evaluation of Environment-specific Force Field for Ordered and Disordered Proteins

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The authors declare that there is no conflict of interest.

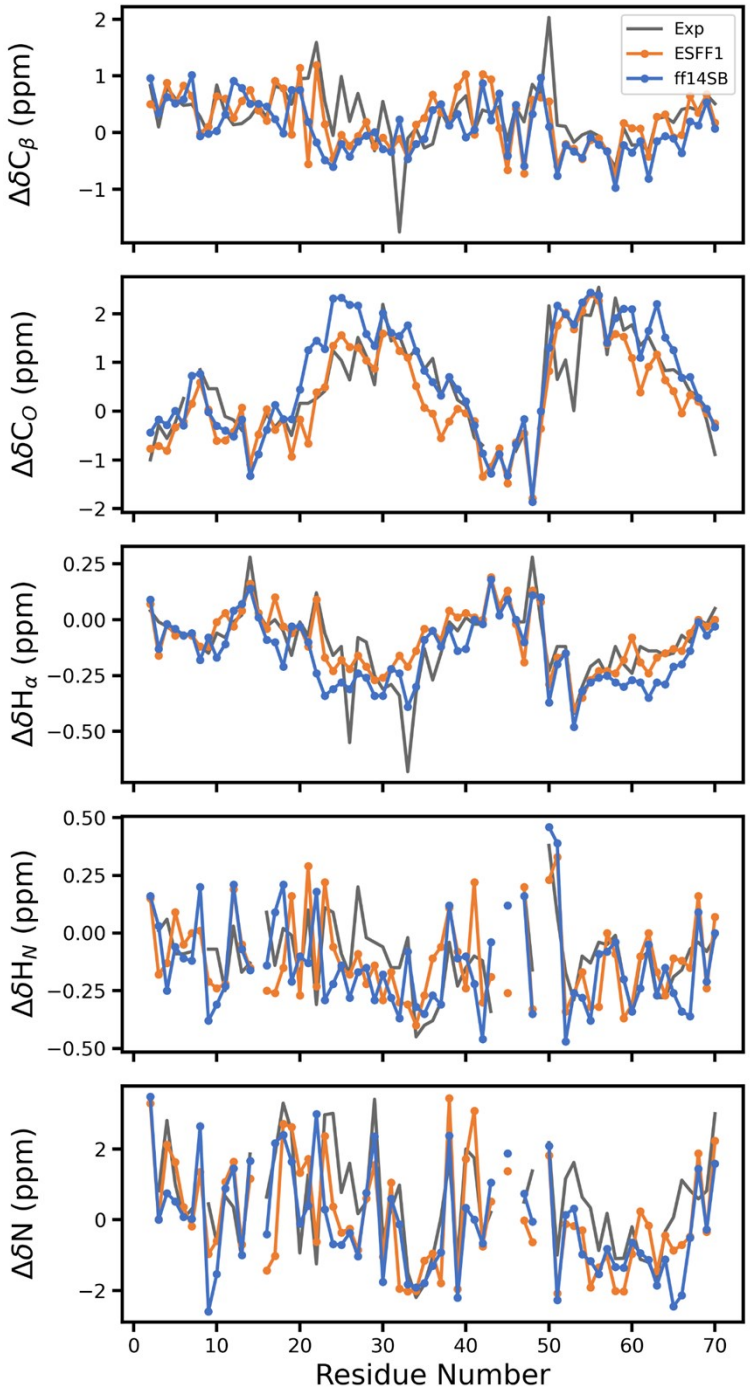

Fig. S1. Comparison of Simulated and experimental chemical shifts of Cβ, C_O, Hα, H_N and N atoms for PaaA2 with ESFF1 and ff14SB force fields.

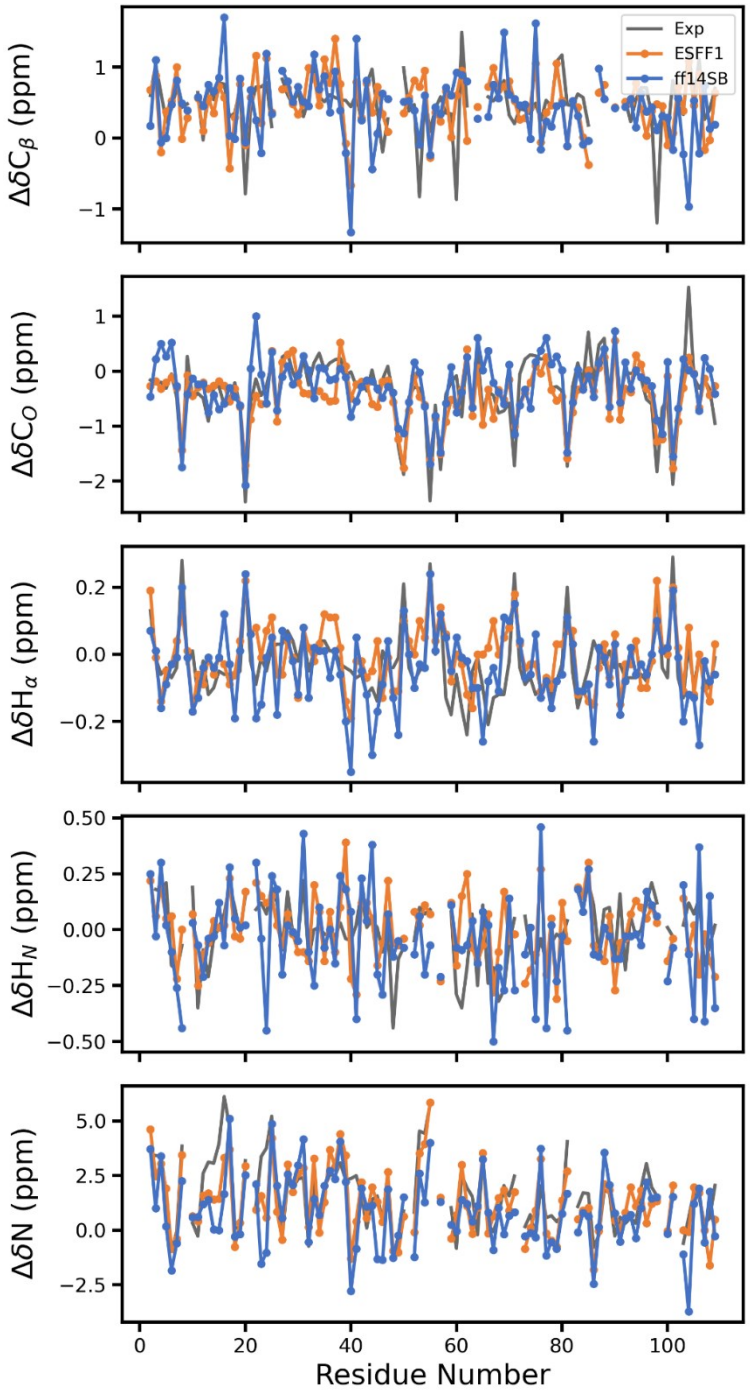

Fig. S2. Comparison of Simulated and experimental chemical shifts of Cβ, C_O, Hα, H_N and N atoms for $p15^{PAF}$ with ESFF1 and ff14SB force fields.

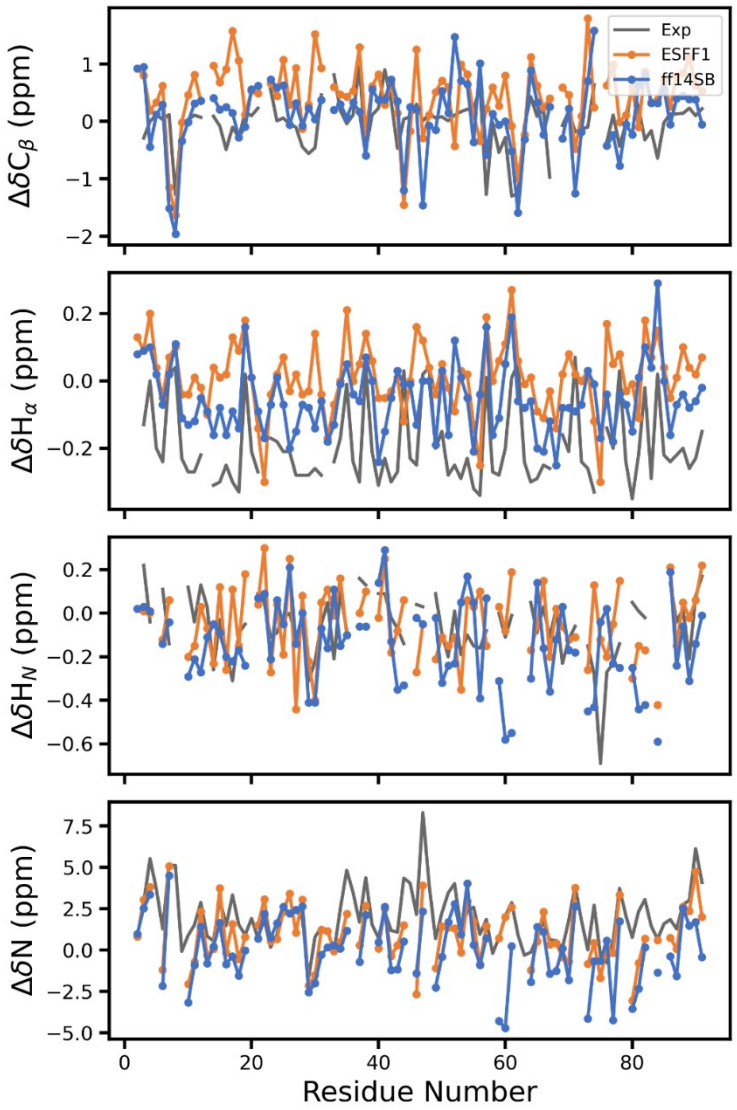

Fig. S3. Comparison of Simulated and experimental chemical shifts of Cβ, Hα, H_N and N atoms for Sic1 with ESFF1 and ff14SB force fields.

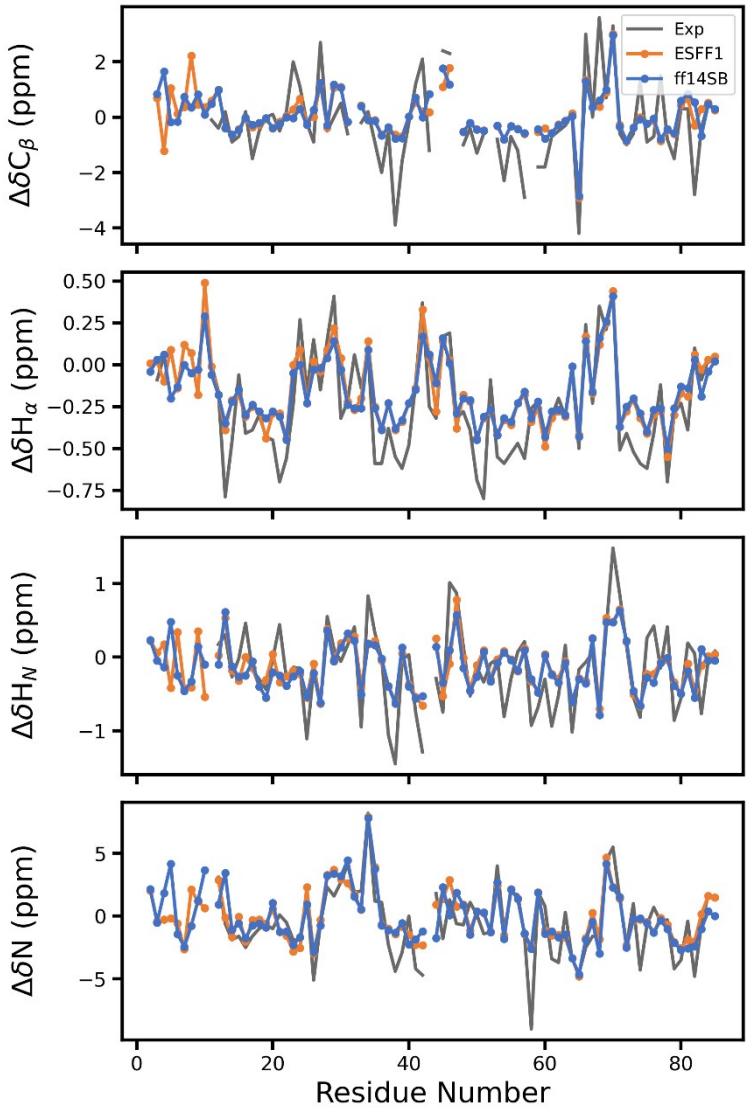

Fig. S4. Comparison of simulated and experimental chemical shifts of Cβ, Hα, H_N and N atoms for ordered protein 2KRK which only has α helix with ESFF1 and ff14SB force fields.

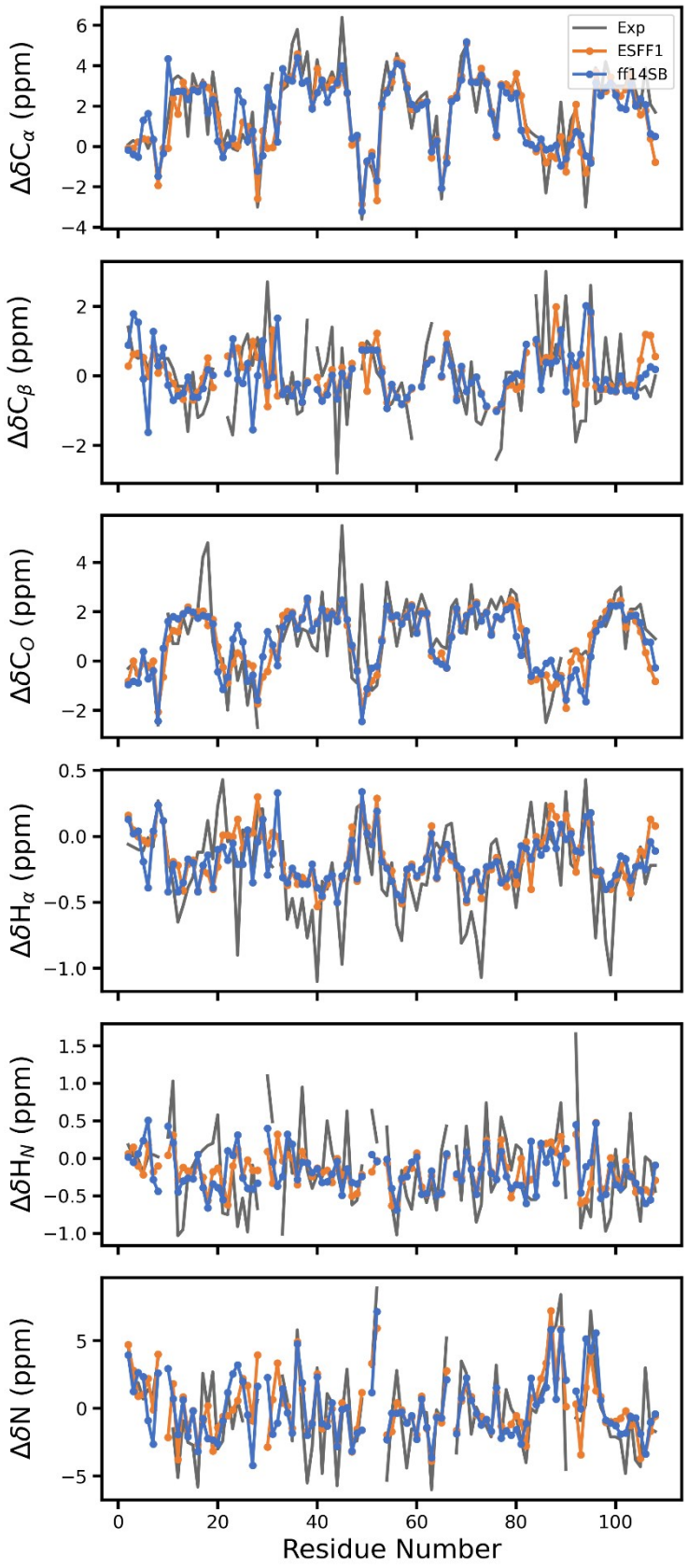

Fig. S5. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_o, Hα, H_N and N atoms for ordered protein 2JN8 which only has α helix with ESFF1 and ff14SB force fields.

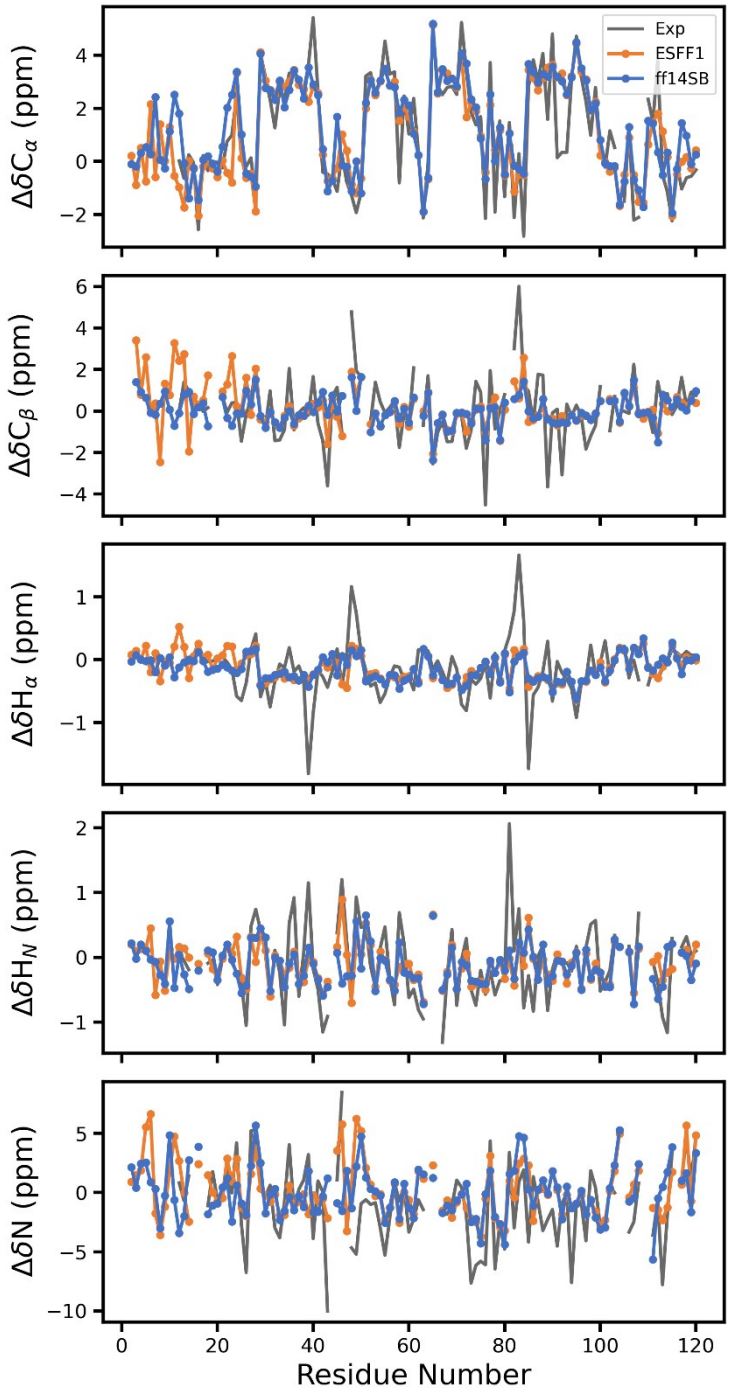

Fig. S6. Comparison of simulated and experimental chemical shifts of Cα, Cβ, Hα, H_N and N atoms for ordered protein 2KHN which only has α helix with ESFF1 and ff14SB force fields.

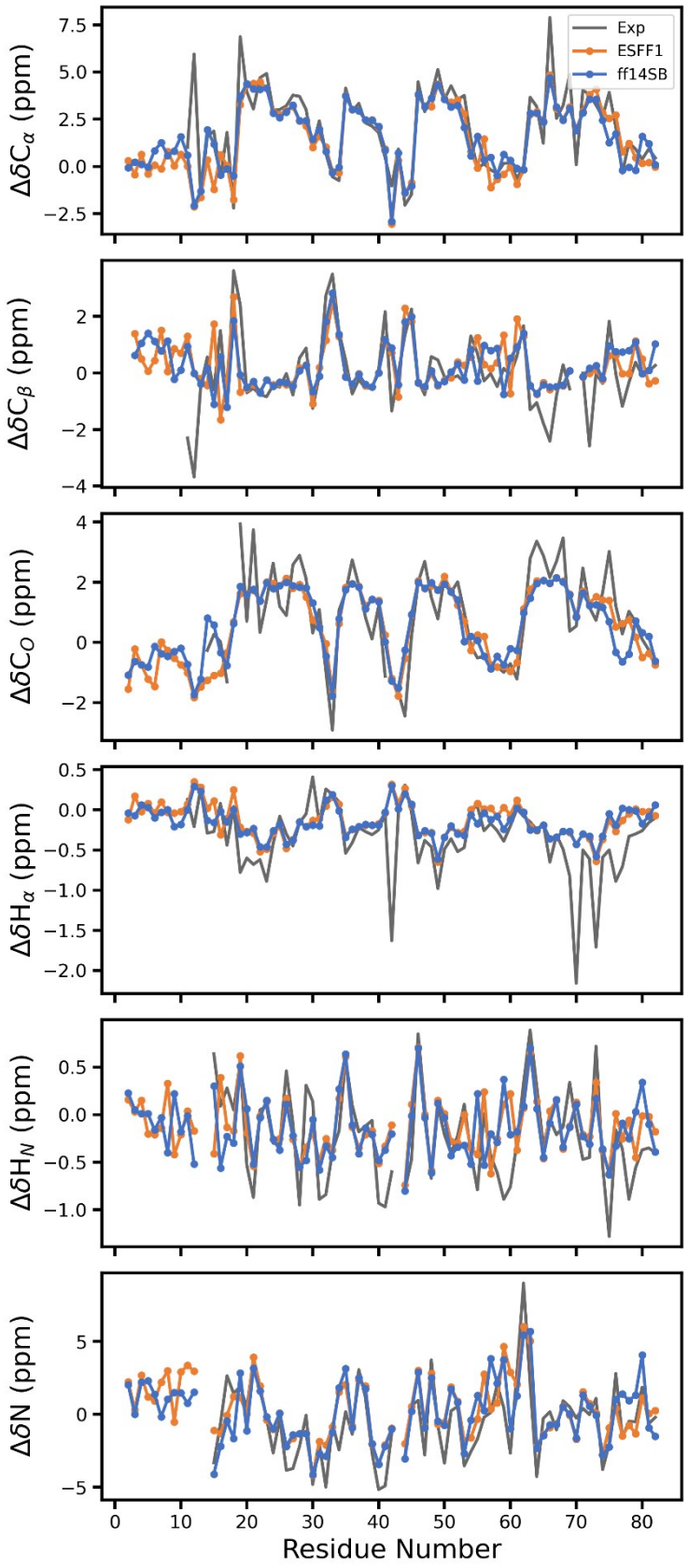

Fig. S7. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 2L1P which only has α helix with ESFF1 and ff14SB force fields.

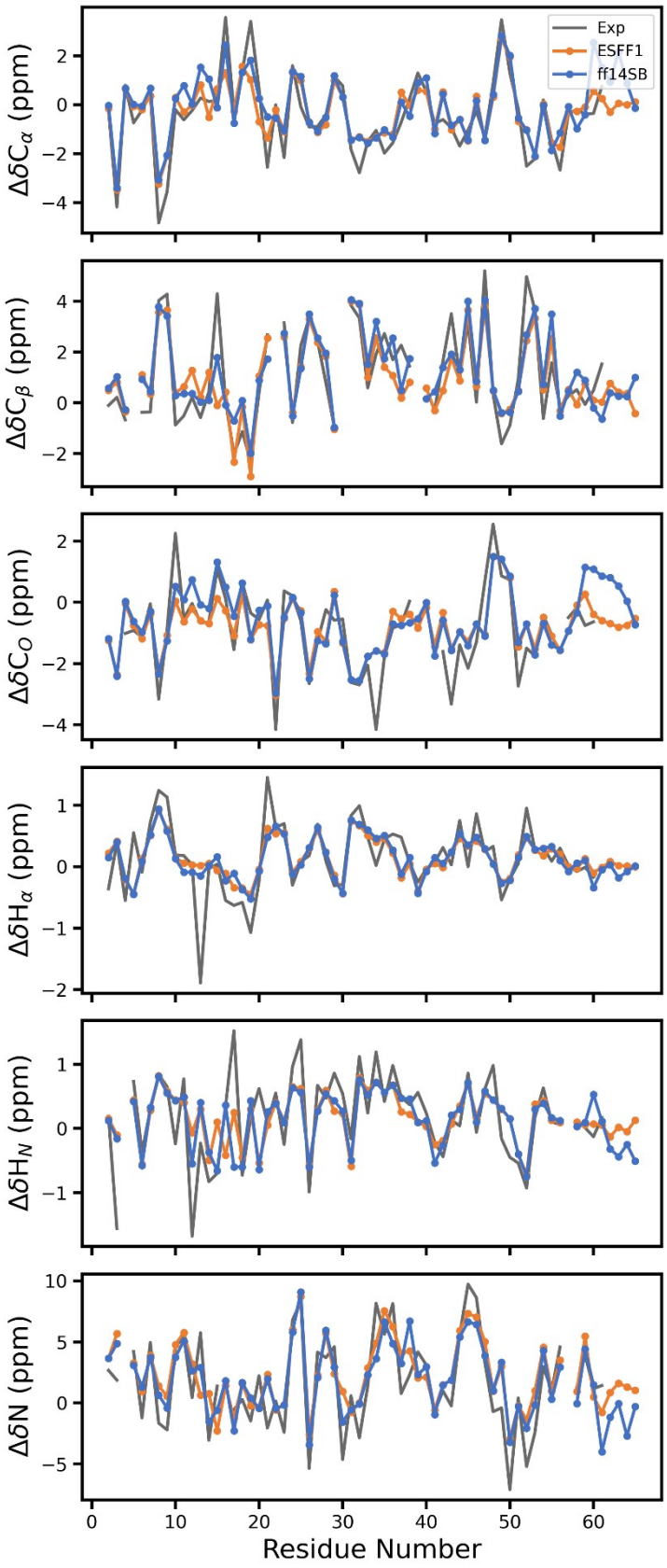

Fig. S8. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 2JZ2 which only has β sheet with ESFF1 and ff14SB force fields.

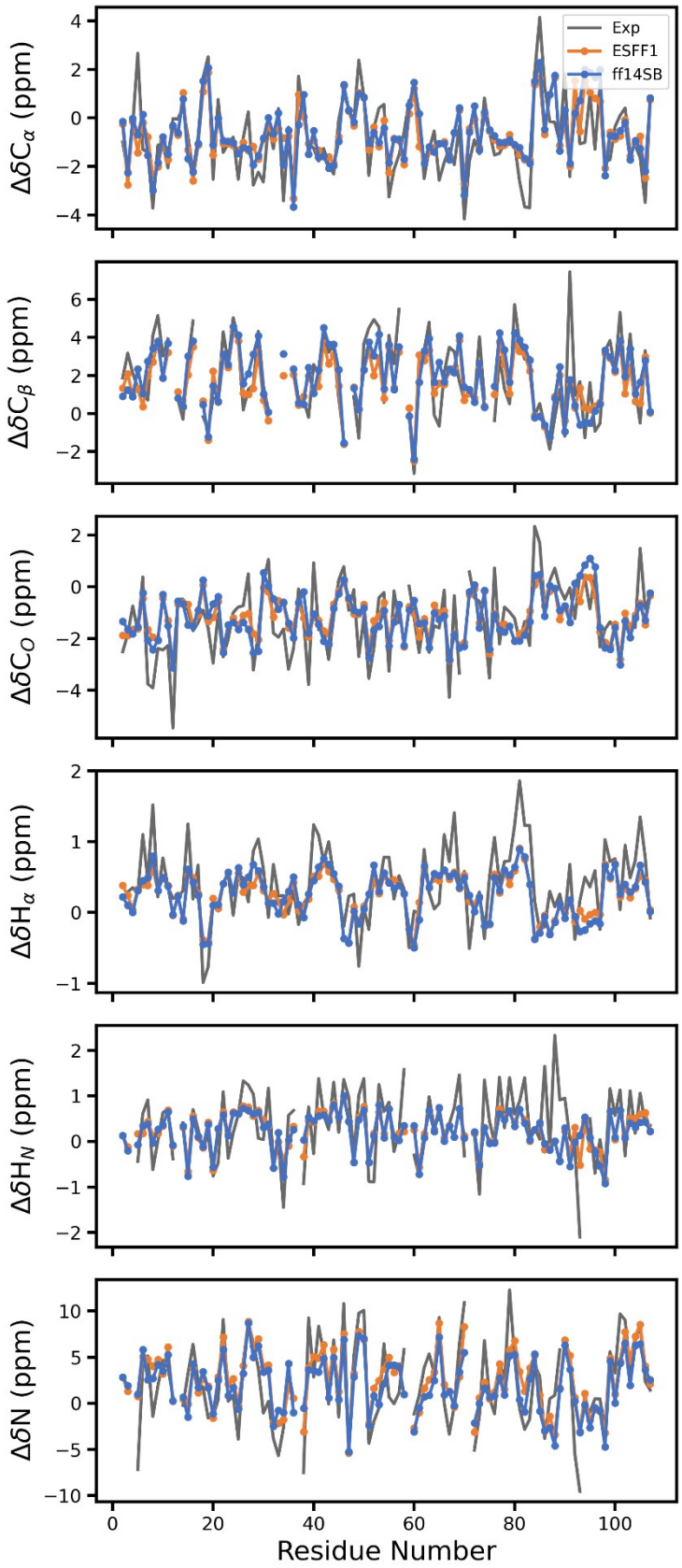

Fig. S9. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 2KL6 which only has β sheet with ESFF1 and ff14SB force fields.

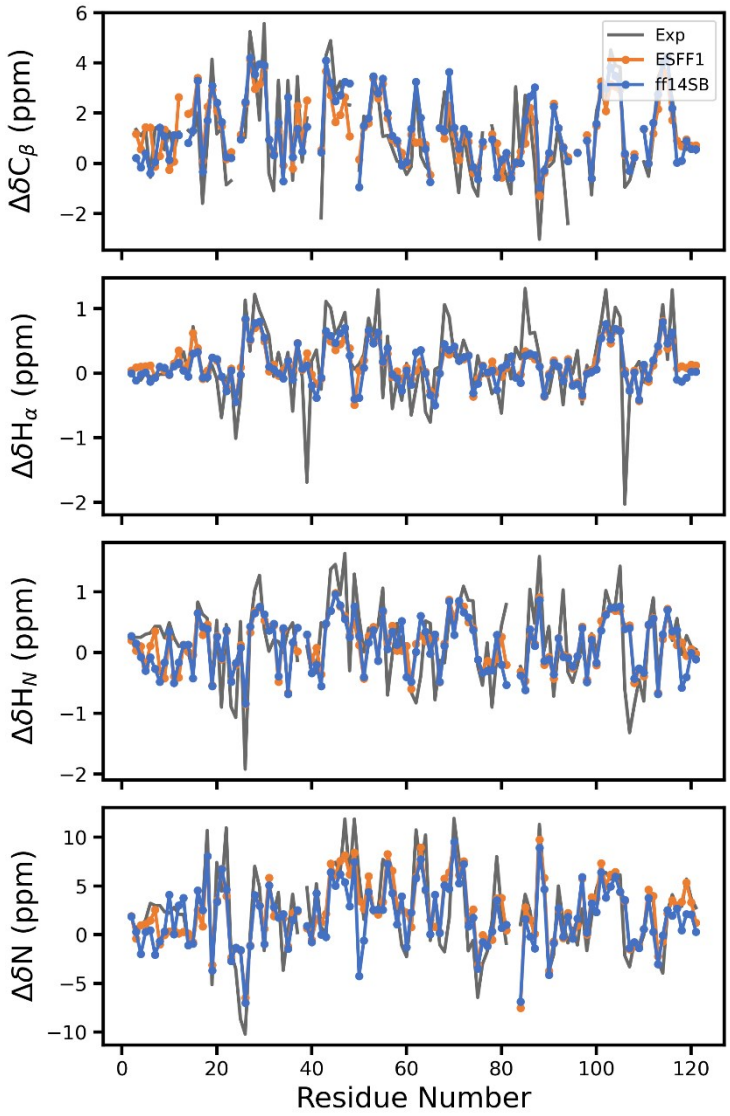

Fig. S10. Comparison of simulated and experimental chemical shifts of Cβ, Hα, H_N and N atoms for ordered protein 2KPW which only has β sheet with ESFF1 and ff14SB force fields.

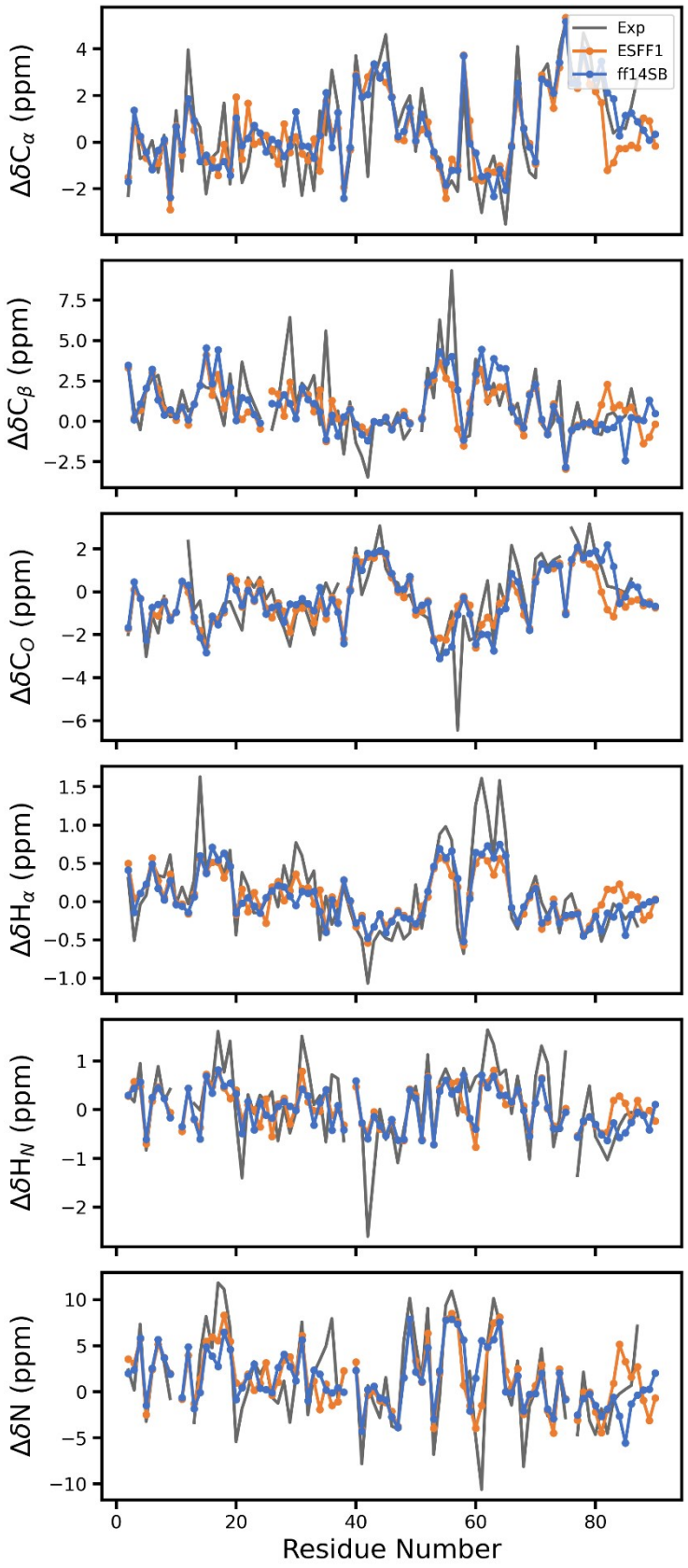

Fig. S11. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 1PQX which both has α helix and β sheet with ESFF1 and ff14SB force fields.

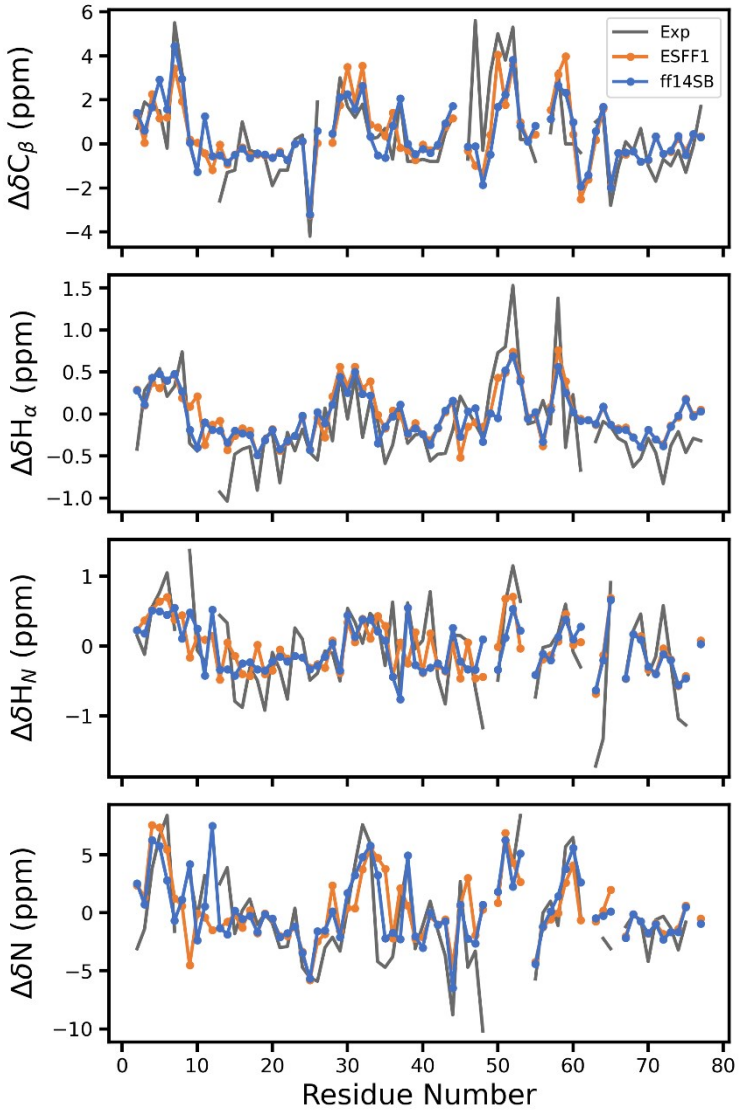

Fig. S12. Comparison of simulated and experimental chemical shifts of Cβ, Hα, H_N and N atoms for ordered protein 1XPV which both has α helix and β sheet with ESFF1 and ff14SB force fields.

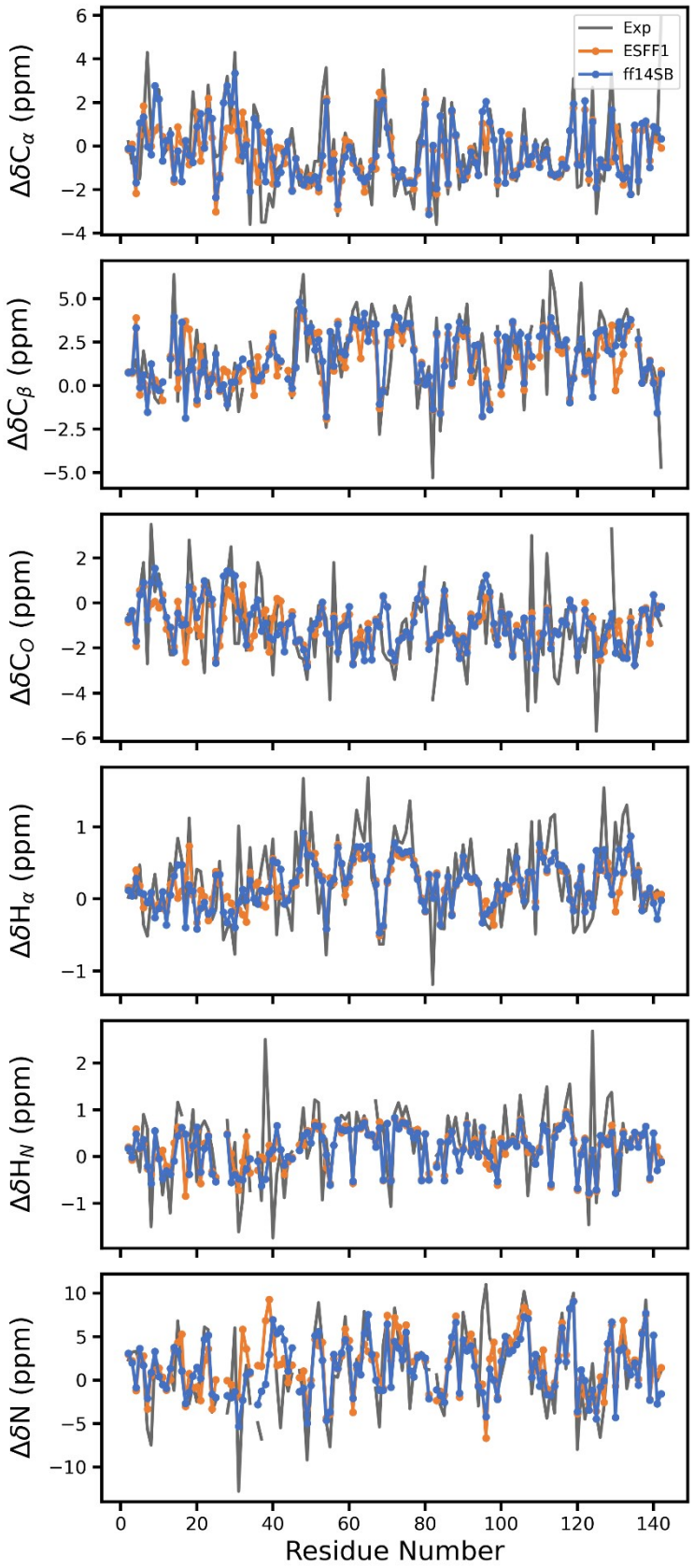

Fig. S13. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 1XPW which both has α helix and β sheet with ESFF1 and ff14SB force fields.

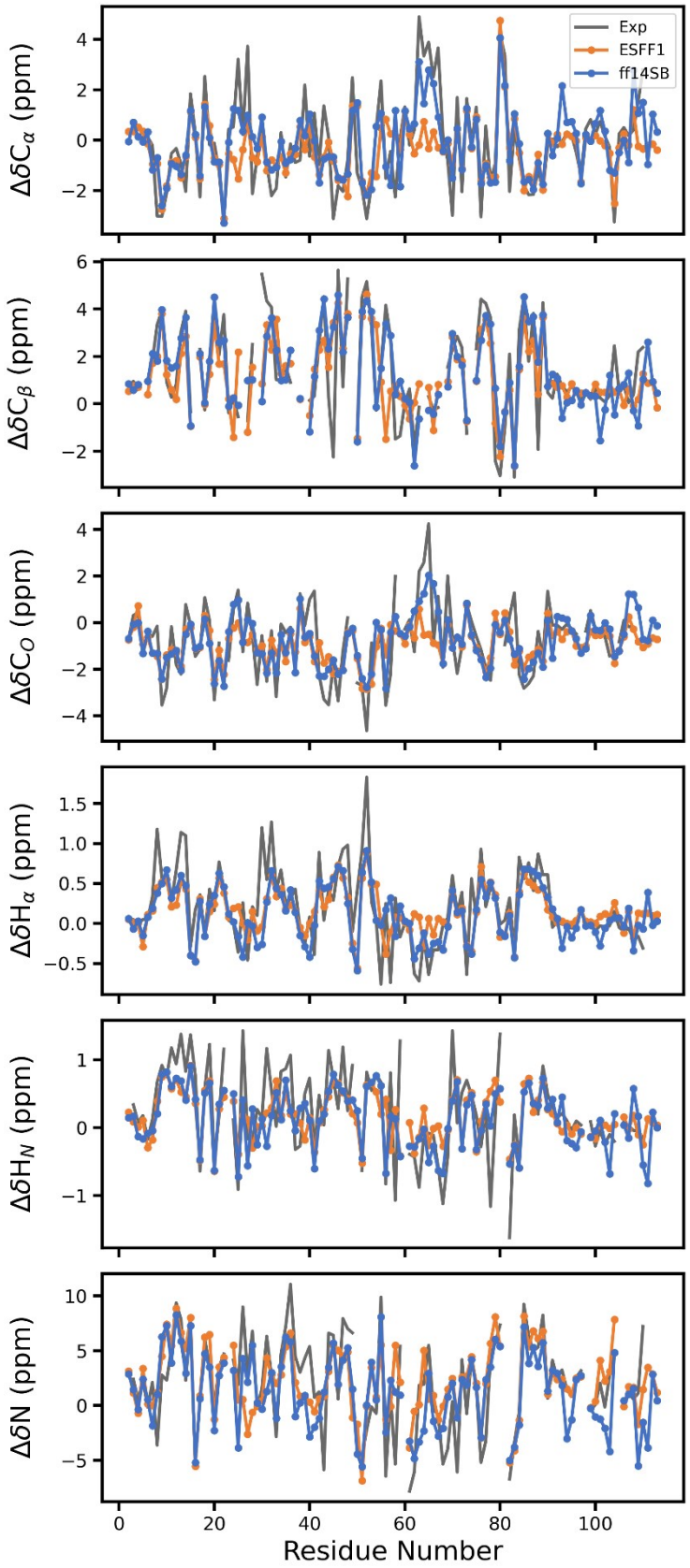

Fig. S14. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N atoms for ordered protein 2KPP which both has α helix and β sheet with ESFF1 and ff14SB force

fields.

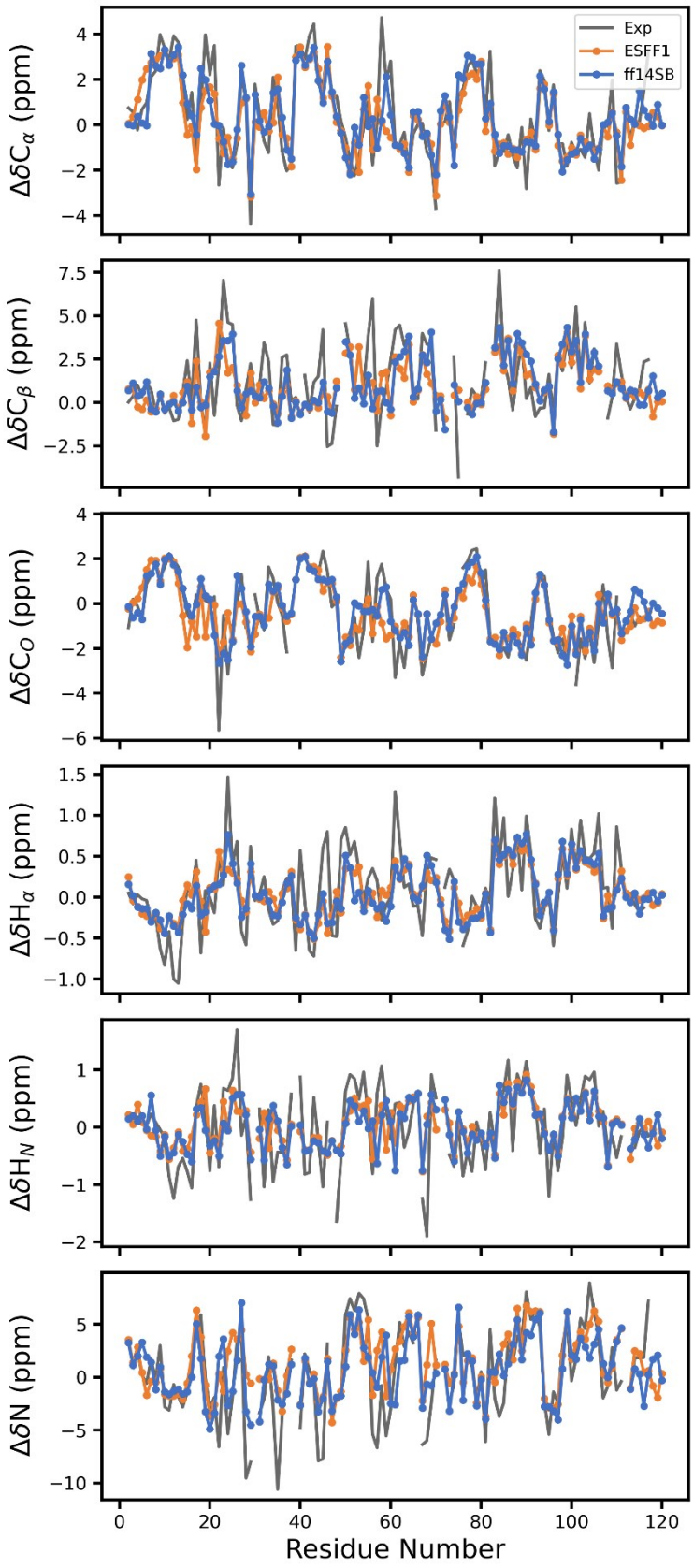

Fig. S15. Comparison of simulated and experimental chemical shifts of Cα, Cβ, C_O, Hα, H_N and N

atoms for ordered protein 2KRT which both has α helix and β sheet with ESFF1 and ff14SB force fields.

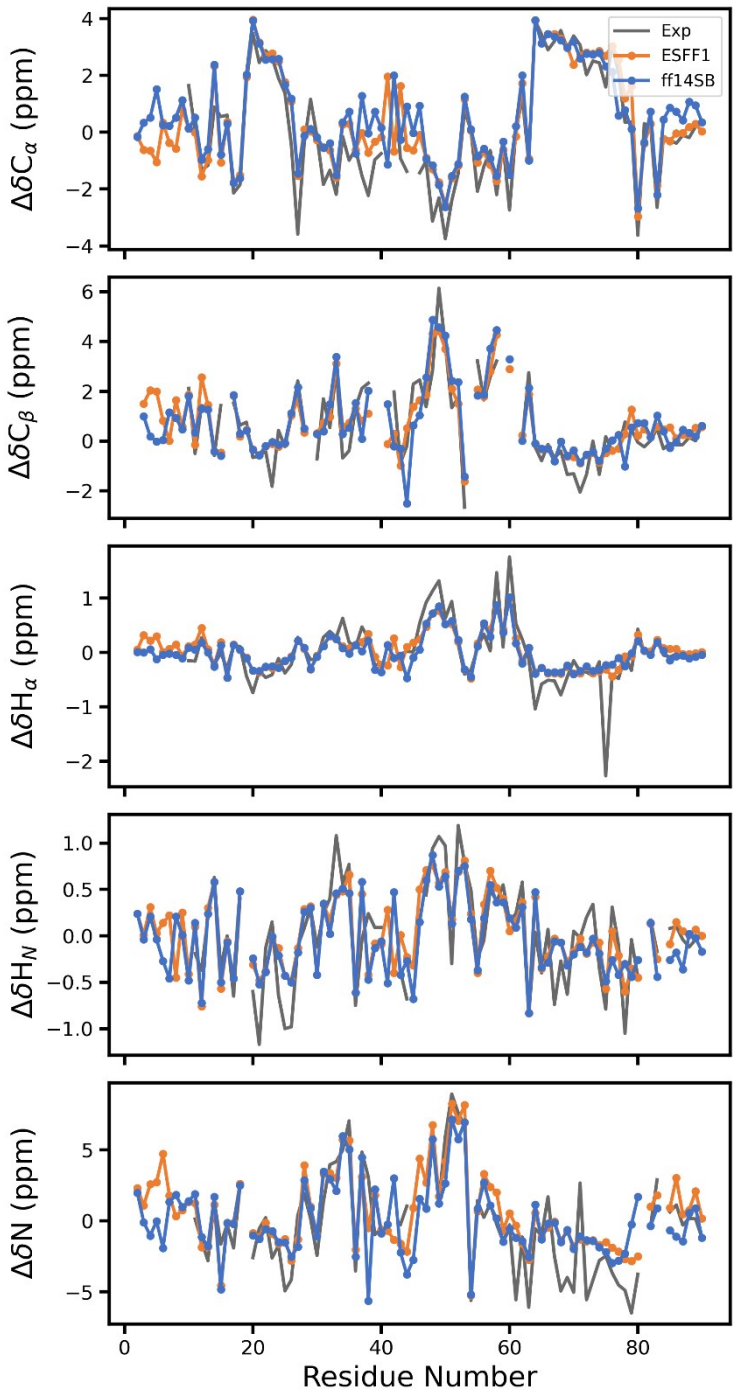

Fig. S16. Comparison of simulated and experimental chemical shifts of Cα, Cβ, Hα, H_N and N atoms for ordered protein 2L33 which both has α helix and β sheet with ESFF1 and ff14SB force fields.

Table S1. The force field score all systems with ESFF1, ff14SB, and the previous study of a99SB-disp.

System	a99SB-disp	ff14SB	ESFF1
PaaA2	1.21	1.36	1.27
p15PAF	1.14	1.51	1.47
Sic1	1.23	2.20	2.03
2KRK	1.06	1.10	1.02
2JN8	1.05	1.12	1.04
2KHN	1.00	1.24	1.22
2L1P	1.00	1.26	1.25
2JZ2	1.06	1.07	1.06
2KL6	1.01	1.11	1.08
2KPW	1.01	1.16	1.16
1PQX	1.10	1.03	1.07
1XPW	1.00	1.14	1.23
1XPV	1.07	1.04	1.14
2KPP	1.00	1.16	1.28
2KRT	1.02	1.02	1.08
2L33	1.01	1.23	1.10