Supporting Information for:

Simulating the distance distribution between spin-labels attached to proteins

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Figure S1. Time dependence of the dihedral angles of $RX_{i,i+4}$ attached to a polyalanine α-helix

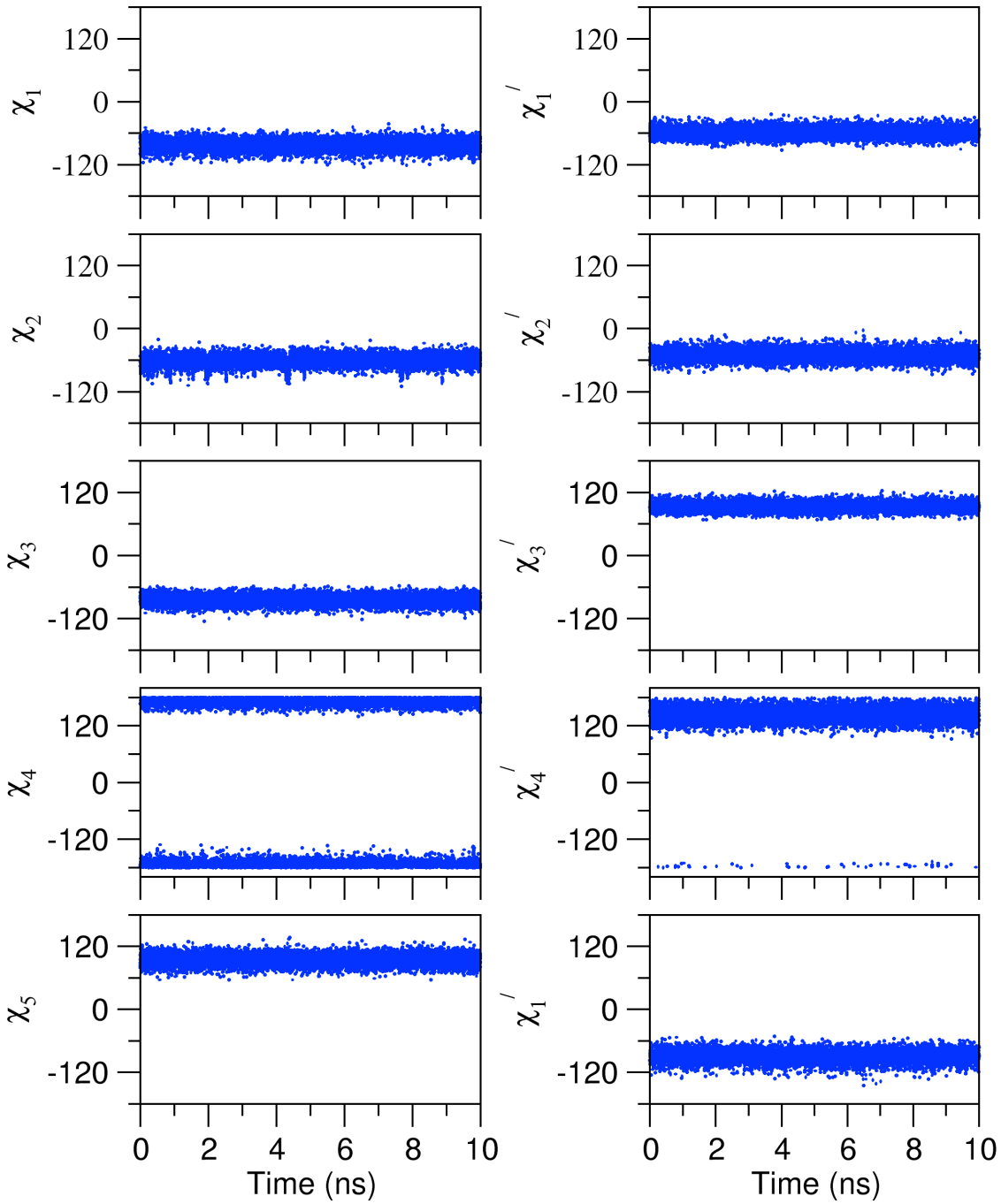


Figure S2. Time dependence of the dihedral angles of $RX_{i,i+3}$ attached to a polyalanine α-helix

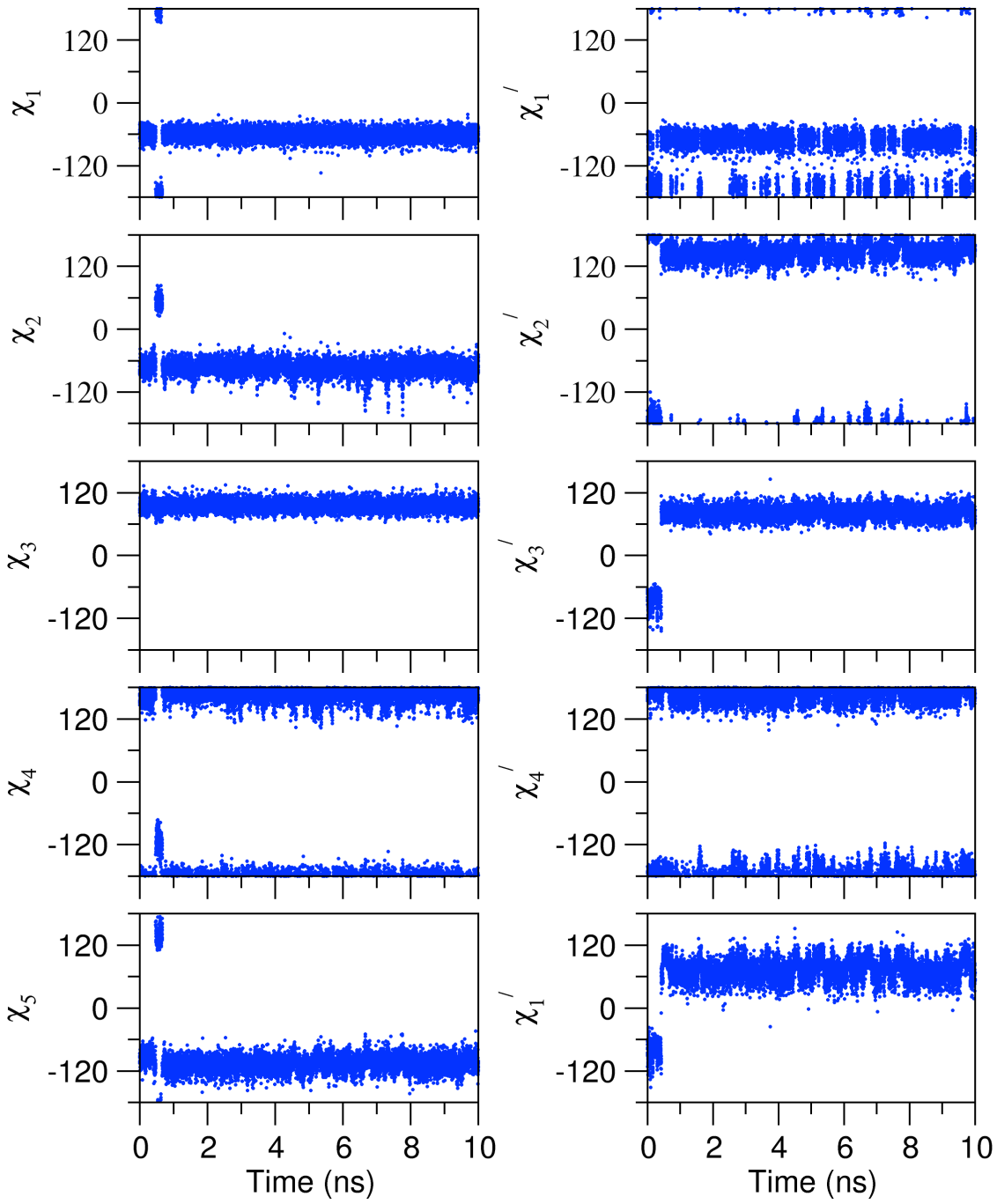


Figure S3. Time dependence of the N-Cα-C-N dihedral angle (ψ) at position i when $RX_{i,i+3}$ is attached to a polyalanine α-helix. In this case, i = 8.

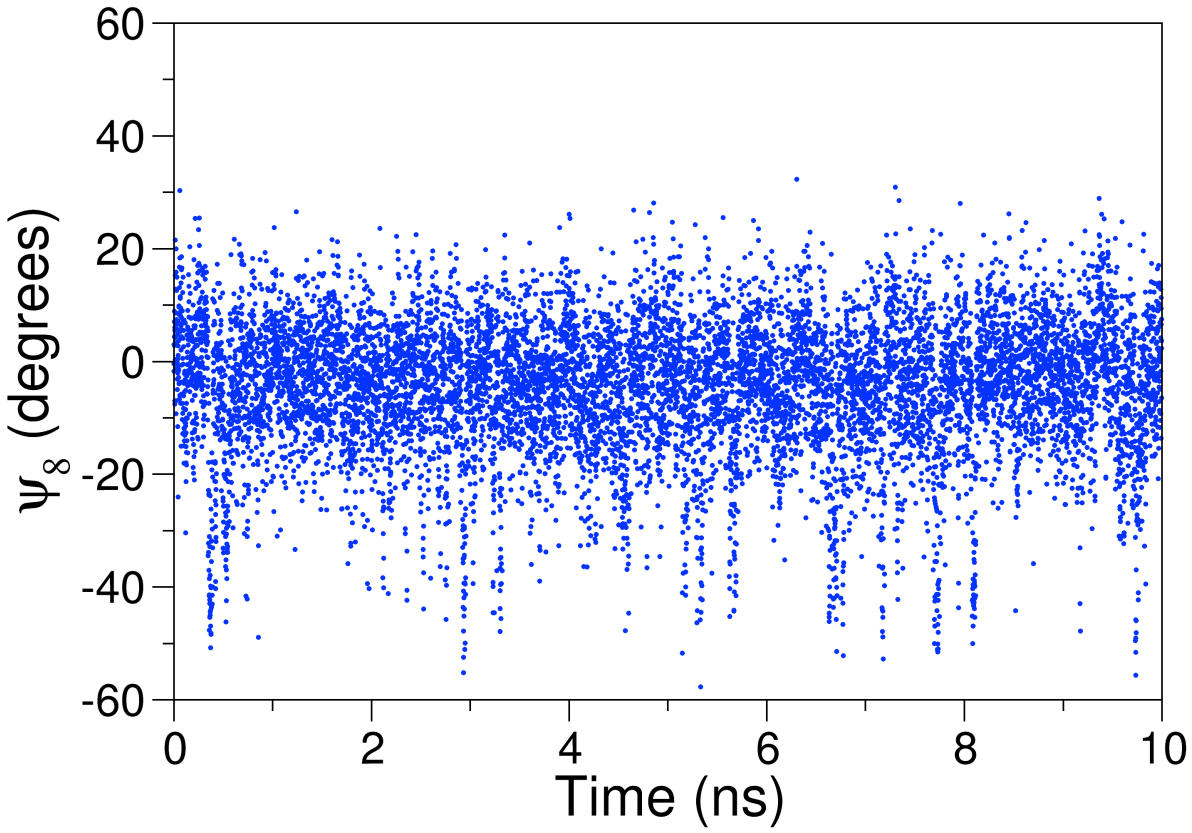


Figure S4. The dynamics of the nitroxide oxygen of the R1 with respect to the Cα atom.

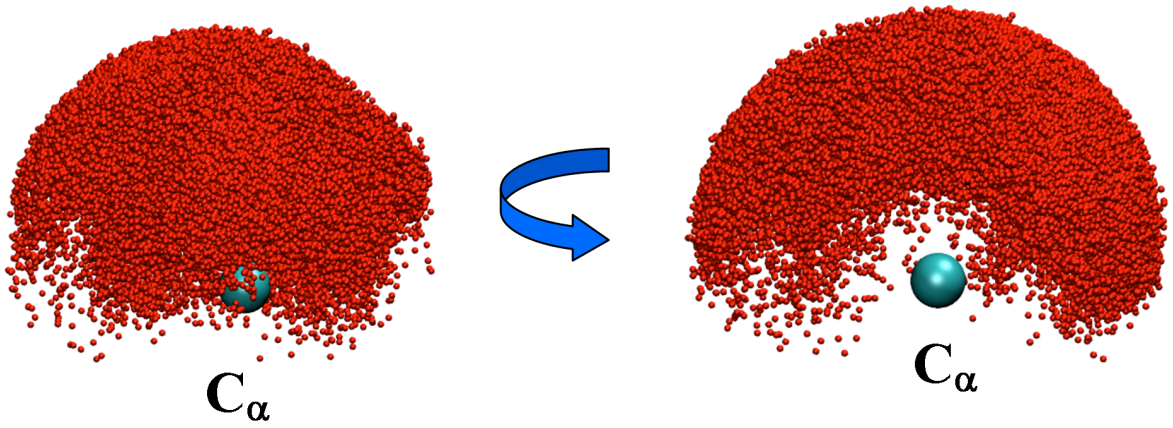


Figure S5. Simplified dummy OND and dummy CBD is attached to Cα atom of Glycine.

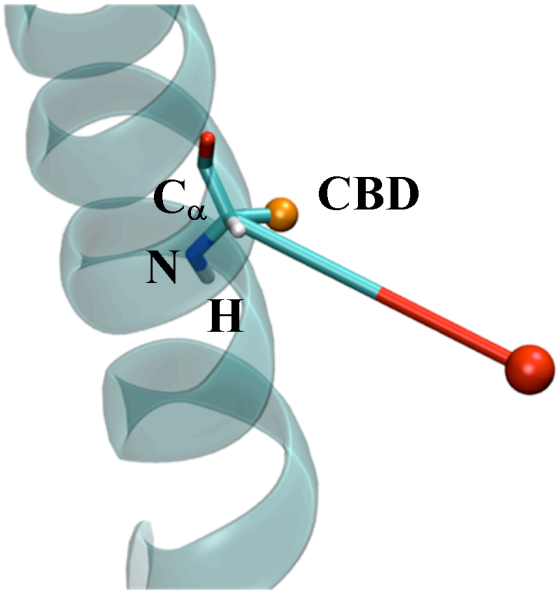
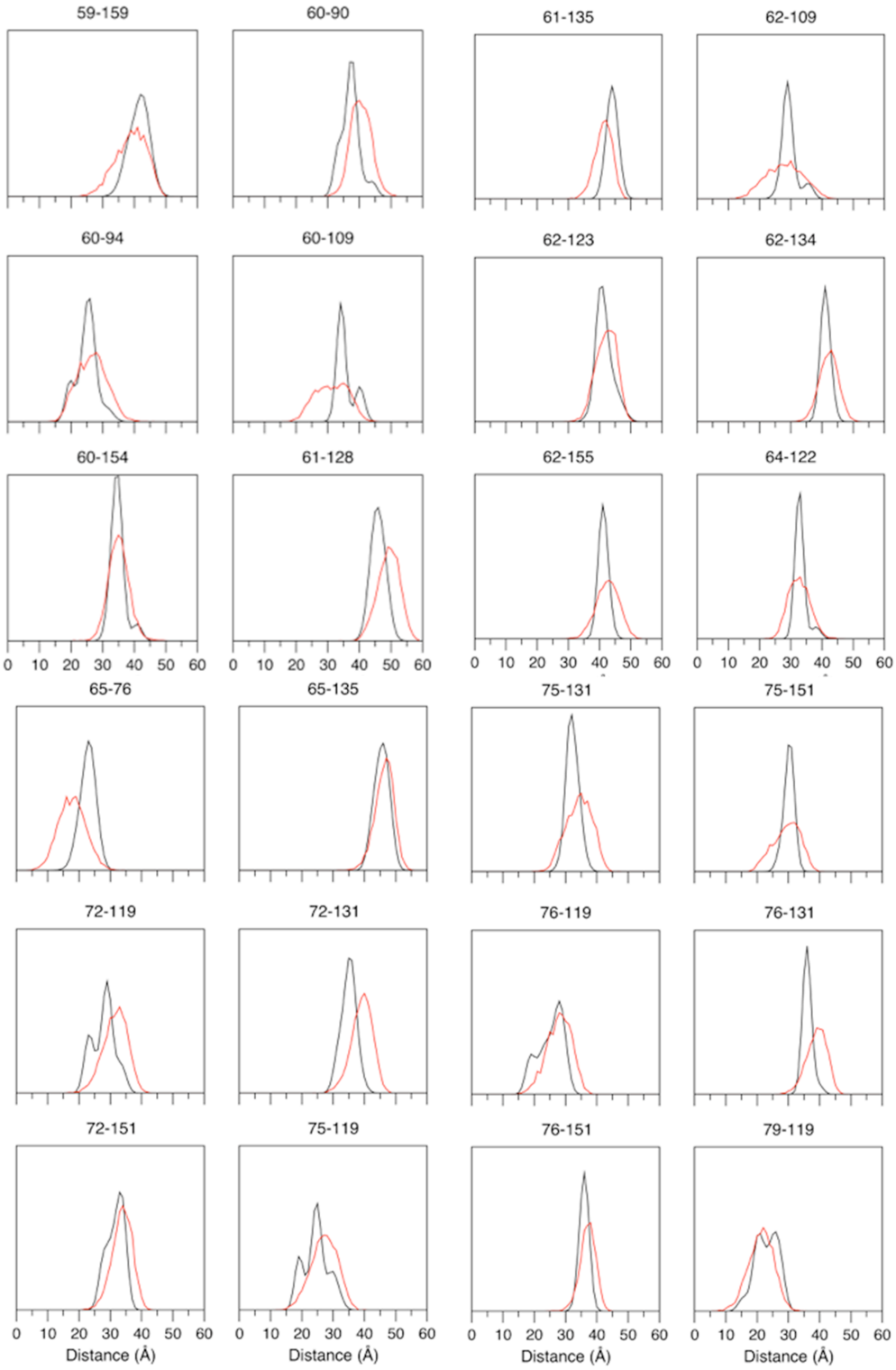


Figure S6. Comparison of the spin-spin distance histograms obtained from 5ns MDDS simulation of T4 lysozyme (red line) and experiment (black line).



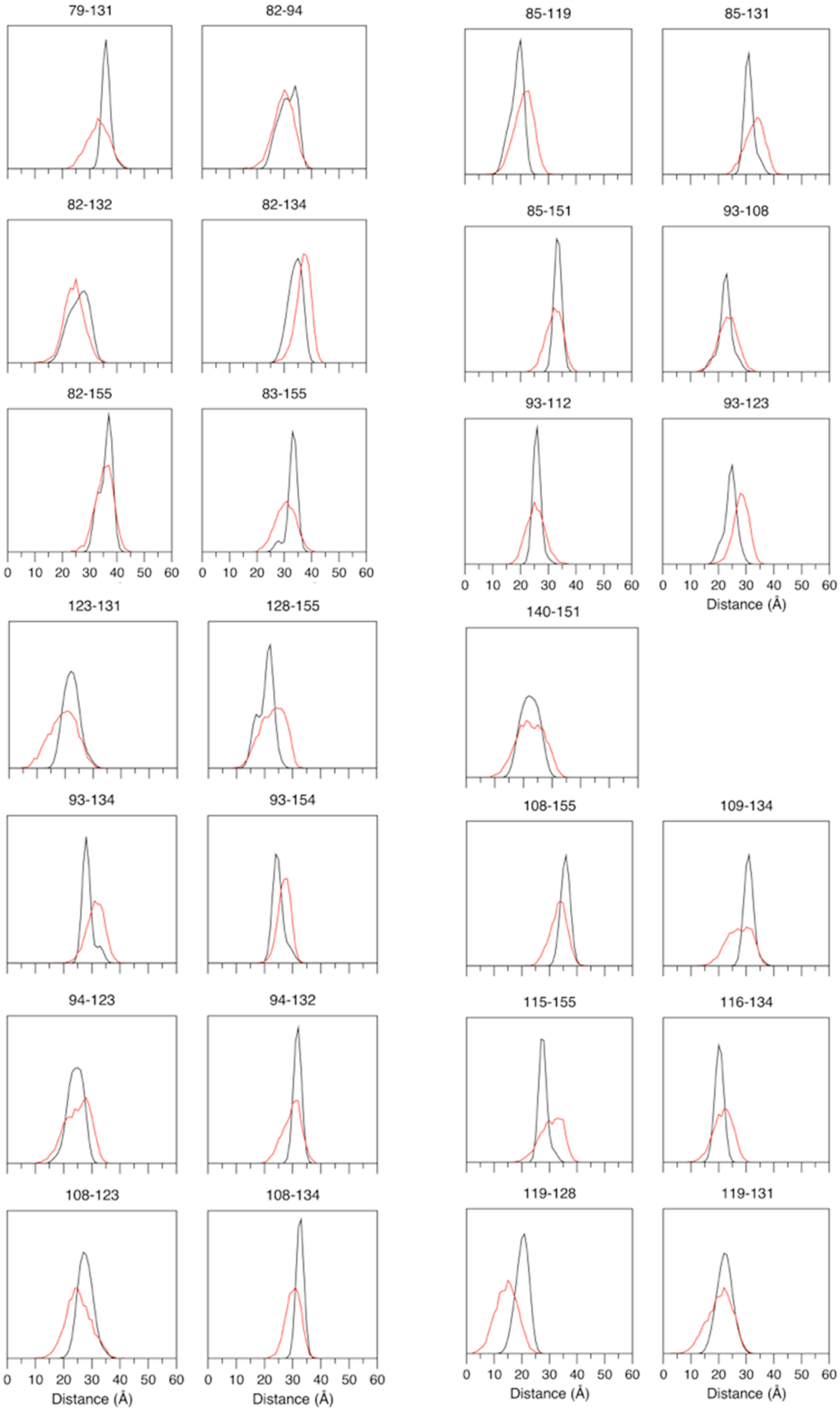

79-131
82-94
85-119
85-131
82-132
82-134
85-151
93-108
82-155
83-155
93-112
93-123
0 10 20 30 40 50 60
Distance (Å)
123-131
128-155
140-151
93-134
93-154
108-155
109-134
94-123
94-132
115-155
116-134
108-123
108-134
119-128
119-131

Table S1: Average spin-pair distances (Å) obtained from DEER, MDDS and MMM and the Cα-Cα distances (Å) obtained from the T4 lysozyme X-ray crystal structure.

Spin-pairs	DEER	MDDS	MMM	CA-CA
59/159	41.12	37.60	38.21	31.25
60/90	37.48	39.66	43.26	35.30
60/94	25.54	22.34	33.37	27.05
60/109	35.15	35.76	34.31	29.35
60/154	34.08	34.26	39.74	33.52
61/128	46.23	48.94	49.08	40.95
61/135	43.92	47.53	45.68	37.66
62/109	29.53	32.43	30.62	26.89
62/123	42.31	48.63	48.17	40.12
62/134	41.06	41.57	45.48	34.46
62/155	41.22	43.38	42.61	34.35
64/122	34.05	32.45	37.64	32.23
65/76	23.18	17.59	17.69	16.80
65/135	45.58	45.23	41.94	34.30
72/119	28.02	30.63	32.75	24.65
72/131	35.57	39.66	37.02	29.18
72/151	31.71	33.54	31.26	23.80
75/119	23.35	24.55	27.92	19.45
75/131	32.76	32.09	32.59	25.13
75/151	30.07	25.32	27.48	20.78
76/119	26.41	27.12	29.16	20.68
76/131	36.52	40.02	36.17	27.76
76/151	36.00	36.57	33.01	24.28
79/119	23.87	21.10	25.05	16.93
79/131	33.06	35.46	33.17	25.81
82/94	30.70	32.09	28.51	21.20
82/132	26.33	24.15	24.67	21.31
82/134	33.89	35.22	30.77	23.68
82/155	35.77	35.63	33.05	25.59
83/155	32.81	30.60	29.60	22.89
85/119	20.01	20.18	19.06	12.28
85/131	31.18	34.80	30.46	22.41
85/151	33.44	31.56	32.23	21.43
93/108	23.28	22.86	26.44	19.11
93/112	26.14	24.49	29.37	19.63
93/123	24.85	27.71	24.13	16.15
93/134	29.15	29.99	28.54	22.03
93/154	25.06	26.44	21.22	13.37
94/123	23.99	28.11	21.87	16.37
94/132	31.73	31.19	26.76	19.55
108/123	27.57	25.84	26.06	20.52
108/134	32.43	29.40	29.42	18.49

108/155	35.23	34.10	31.92	23.32
109/134	30.57	28.95	26.66	18.14
115/155	28.30	31.52	26.43	20.60
116/134	20.16	20.65	17.14	11.94
119/128	19.93	15.48	14.91	10.42
119/131	22.34	23.84	18.05	13.20
123/131	22.33	22.83	18.81	14.61
128/155	20.69	22.01	16.01	12.08
140/151	22.20	21.61	18.66	15.54

Figure S7. Comparison of distance distributions obtained from MDDS (solid lines) and DEER (dashed line) based on the “outward-facing (3TT1)”(blue), “substrate-occluded (2A65)”(green) and “inward-facing (3TT3)”(red) crystal structures of LeuT.

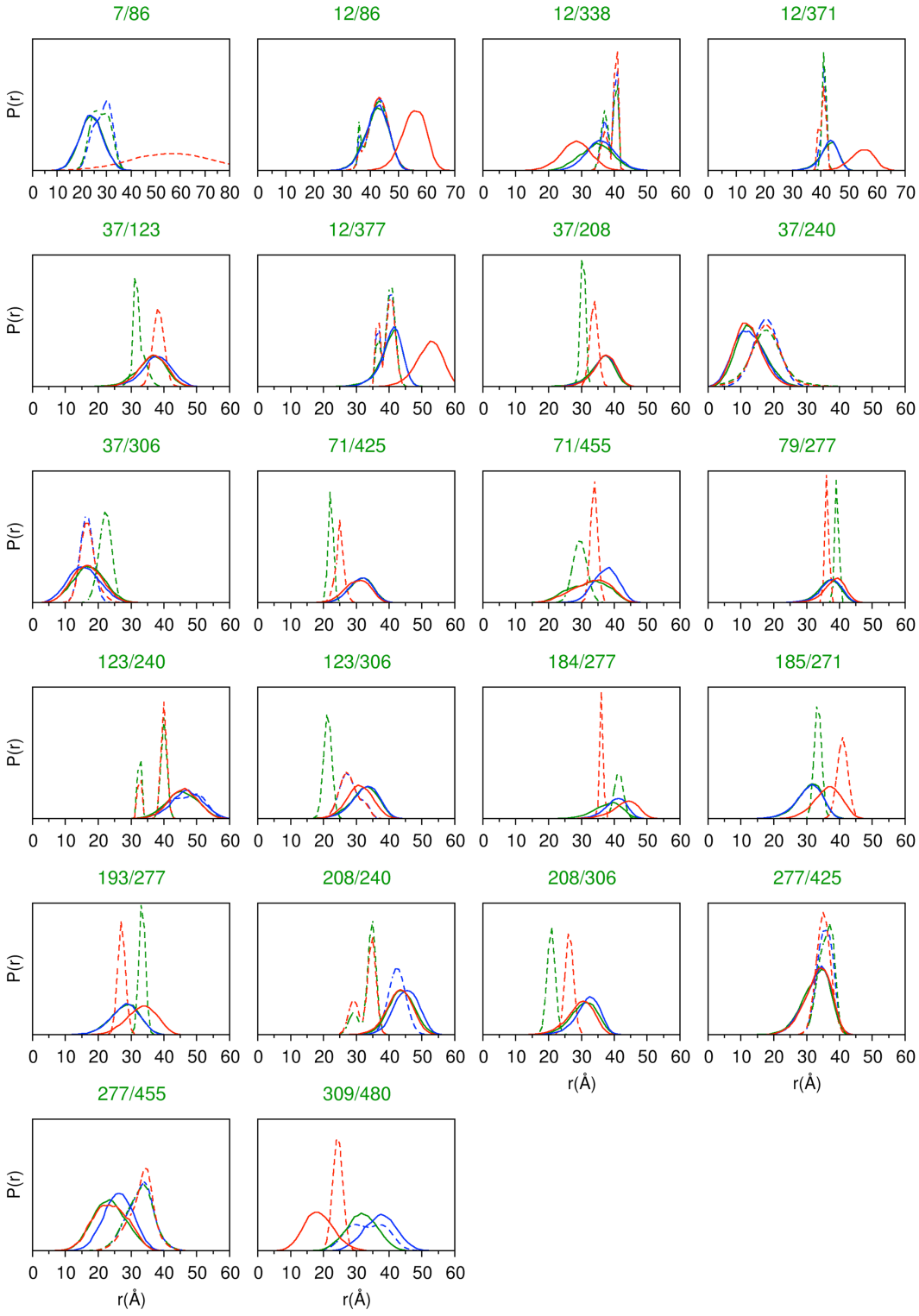


Figure S8. Comparison of DEER, MDDS and re-MD distance distributions between the 109-113RX and 127-131RX attached to T4 lysozyme.

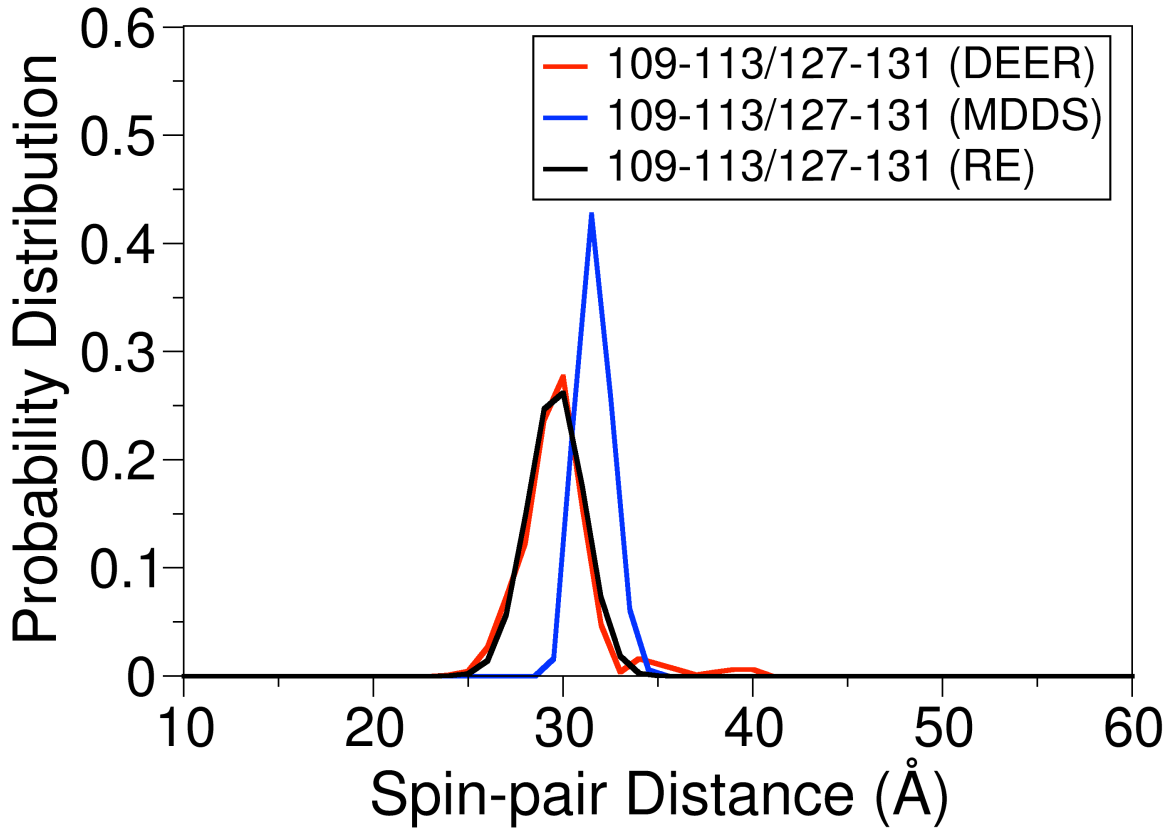


Figure S9. Time dependence of the dihedral angles of $RX_{i,i+4}$ attached to a polyalanine α-helix obtained from 100ns simulation.