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

Supporting information for article

Capturing a dynamically interacting inhibitor by paramagnetic NMR spectroscopy

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Additional tables

Table S1. Distances (in Å) between Fe(III) metal atom and backbone N atoms averaged over MD trajectory.

		average Fe-N distance		restrained Fe-N distance
residue	chain	FREE	DR	DR
27	A	13.9	8.6	19
28	A	13.0	7.5	19
29	A	14.5	8.5	19
30	A	16.3	9.9	19
47	A	11.5	9.6	12
48	A	8.4	6.5	12
49	A	5.5	5.1	12
50	A	7.7	7.5	12
51	A	9.7	10.2	12
52	A	9.8	10.2	12
53	A	8.2	9.5	12
54	A	9.1	10.4	12
82	A	14.5	12.4	19
27	B	13.8	10.0	19
28	B	11.7	8.8	19
29	B	11.9	10.8	19
30	B	11.9	12.3	19
47	B	8.7	9.9	12
48	B	6.6	6.6	12
49	B	7.0	5.5	12
50	B	9.9	6.4	12
51	B	11.3	8.3	12
52	B	11.0	9.6	12
53	B	8.9	9.1	12
54	B	7.8	9.3	12
82	B	8.7	8.9	19

Additional figures

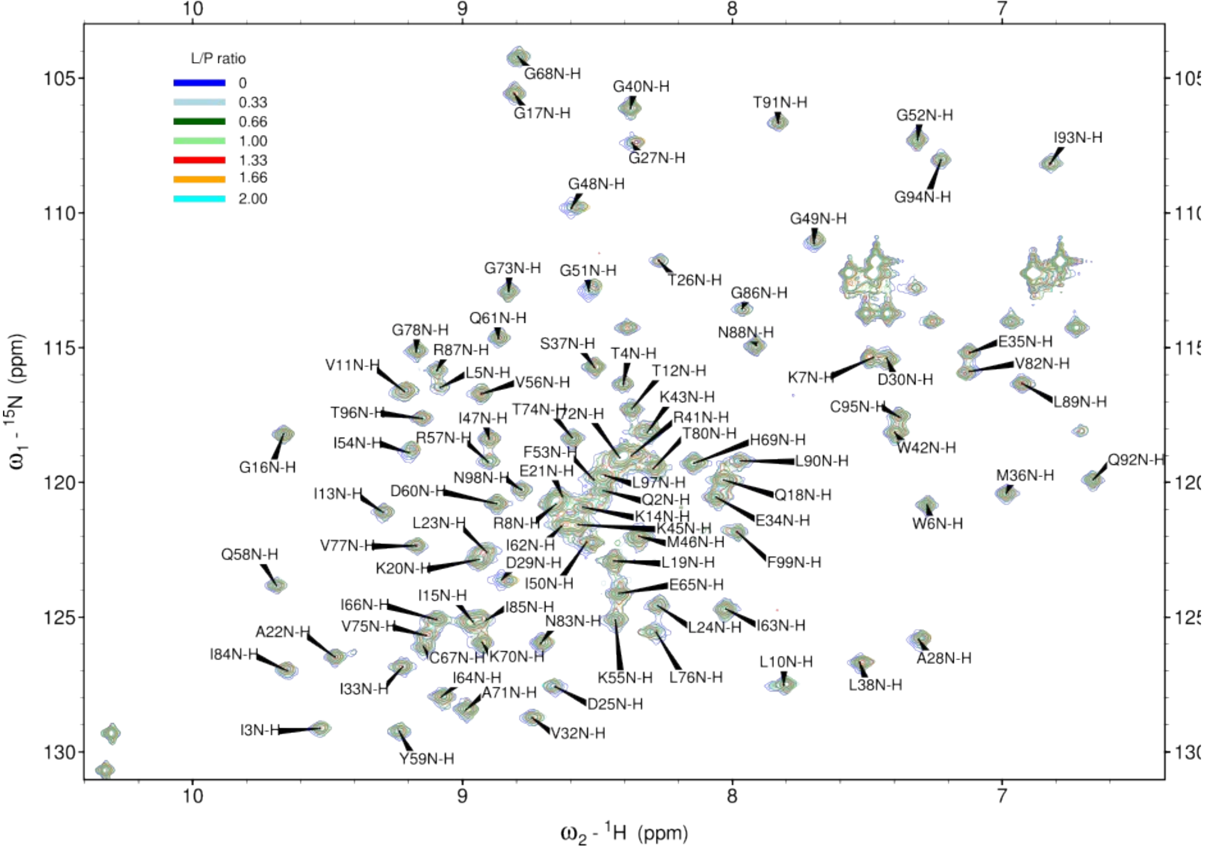

Figure S1. HN HSQC spectra obtained during titration with the diamagnetic ligand.

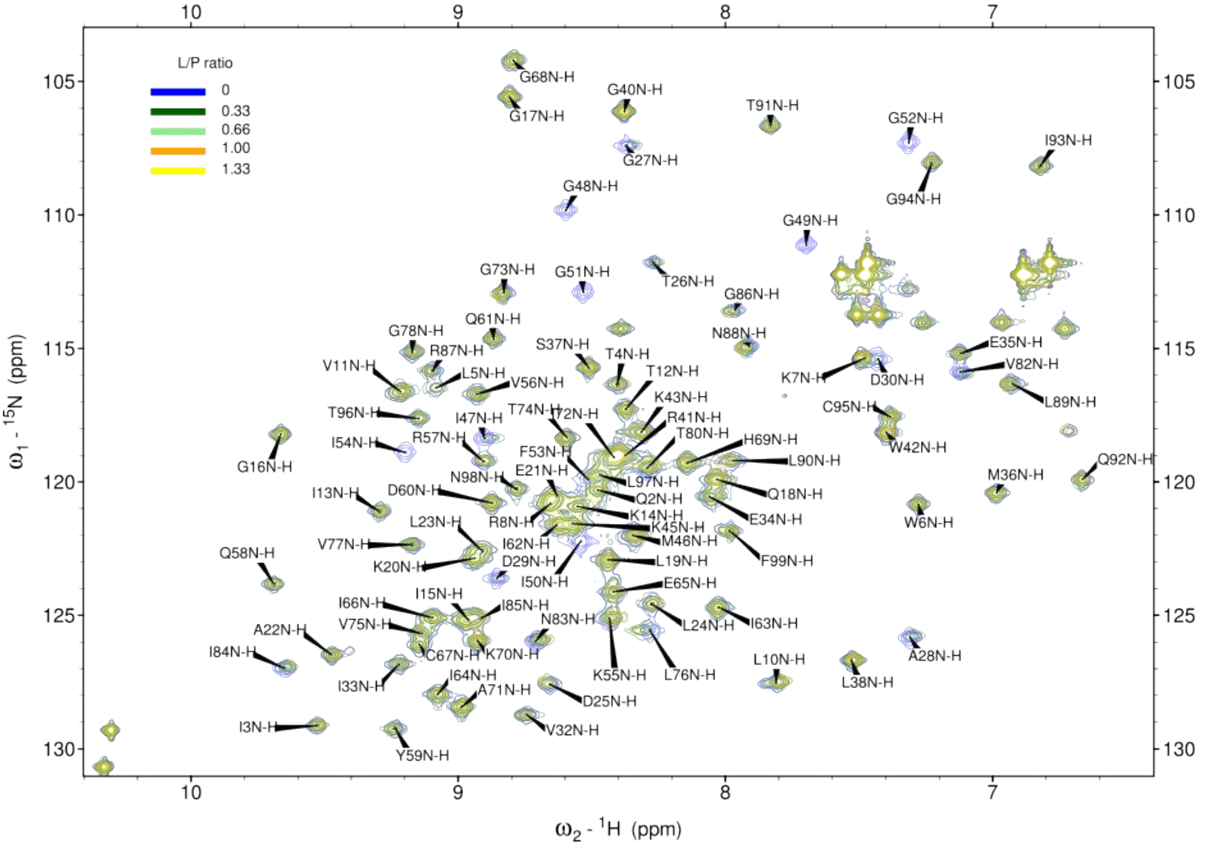

Figure S2. HN HSQC spectra obtained during titration with the paramagnetic ligand.

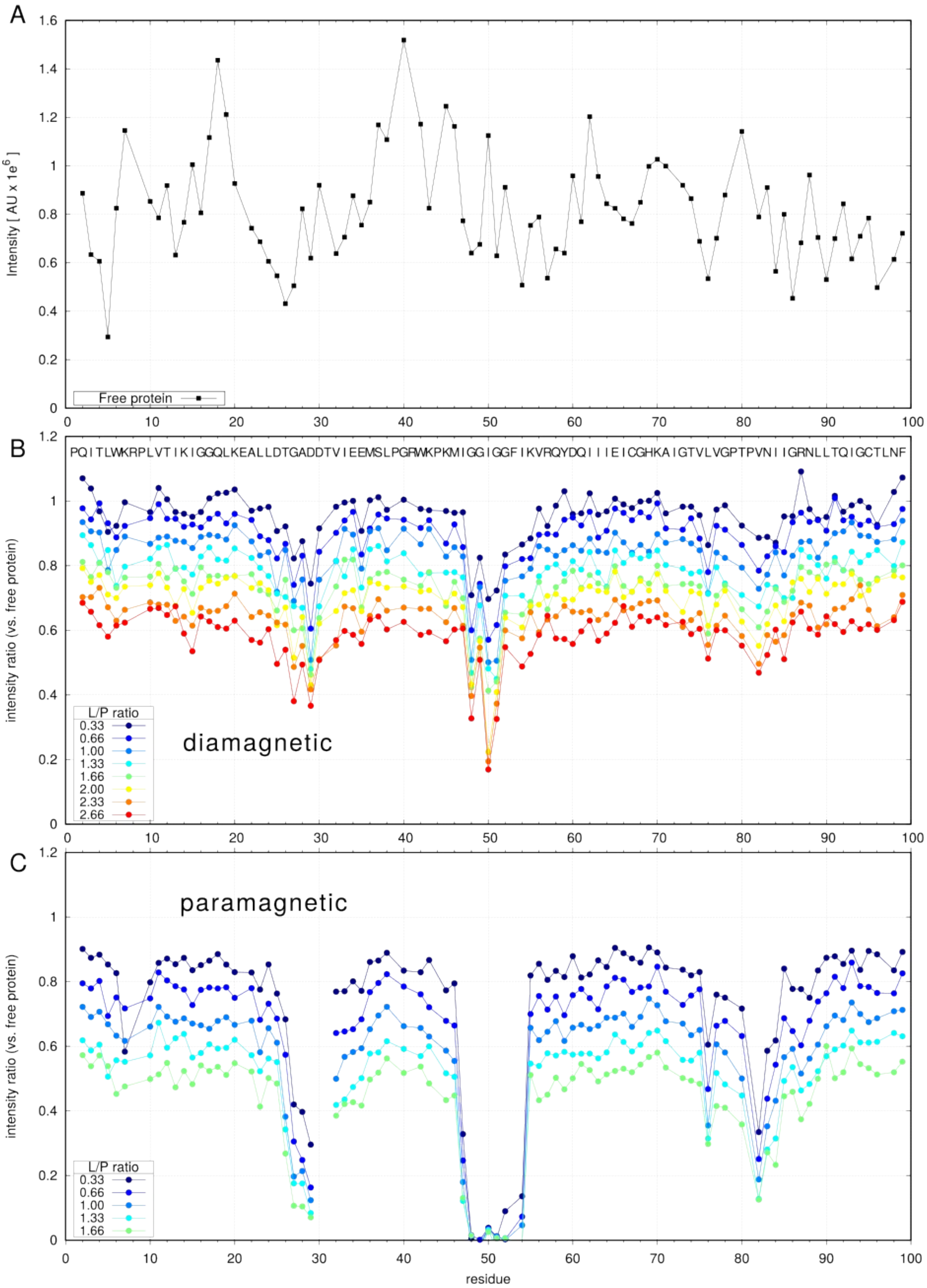

Figure S3. A) NMR signal intensities in HN HSQC spectrum of a free protein. B) intensity ratio of the individual titration steps vs. free protein during – diamagnetic sample. C) intensity ratio of the individual titration steps vs. free protein during – paramagnetic sample.

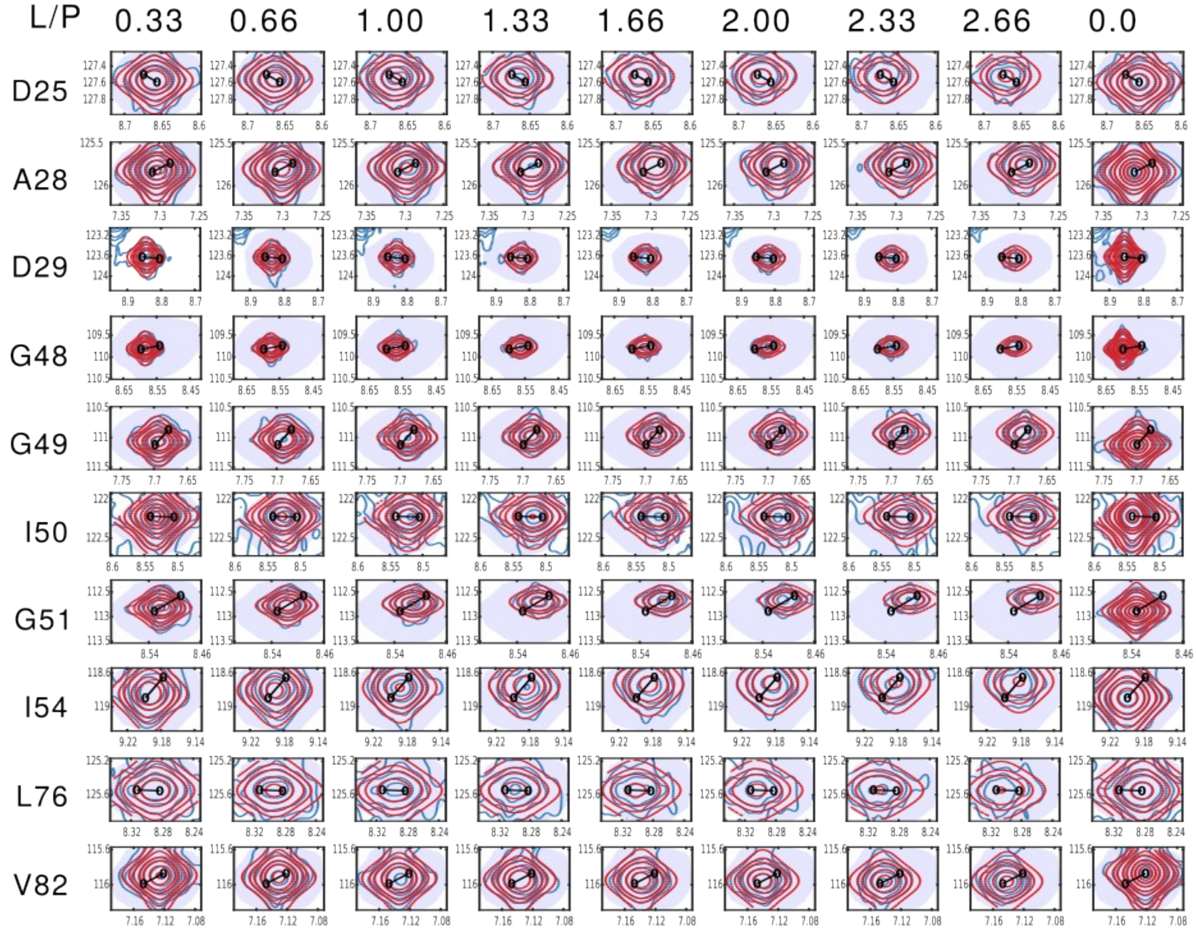

Figure S4. Observed (blue) and fitted (red) signals upon titration of HIV-1 protease with the diamagnetic ligand. Fitted line-shapes are a result of the TITAN analysis.

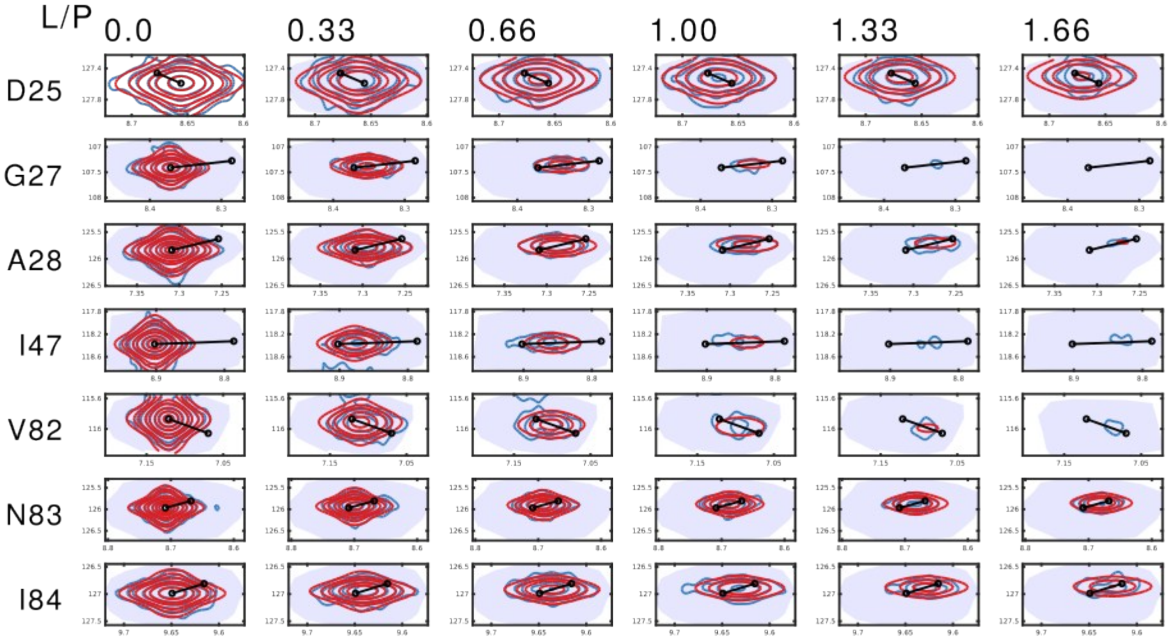

Figure S5. Observed (blue) and fitted (red) signals upon titration of HIV-1 protease with the paramagnetic ligand. Fitted line-shapes are a result of the TITAN analysis.

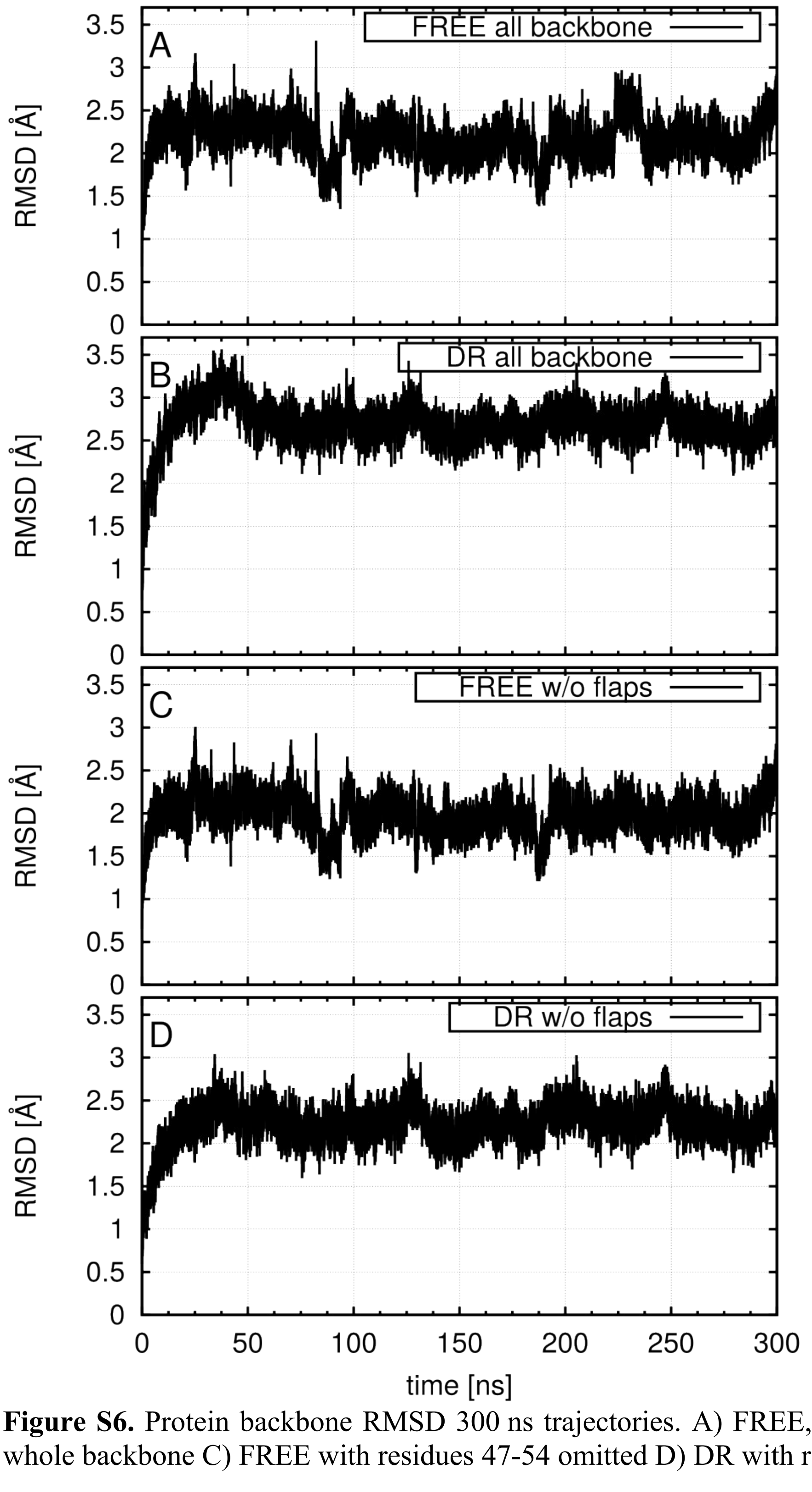

Figure S6. Protein backbone RMSD 300 ns trajectories. A) FREE, whole backbone B) DR, whole backbone C) FREE with residues 47-54 omitted D) DR with residues 47-54 omitted

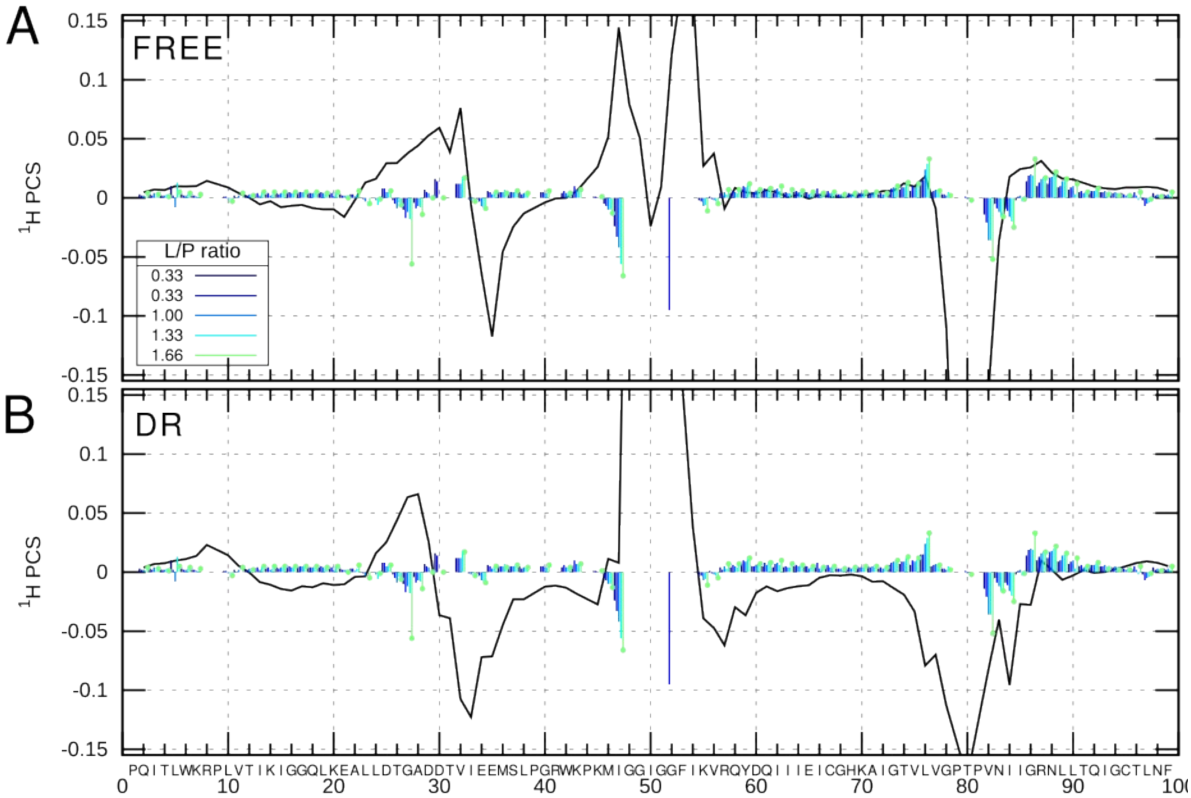

Figure S7. Calculated PCS values for a single snapshot (corresponding to the average structure shown in the Fig. 3) from MD simulation vs. the experimental PCS.

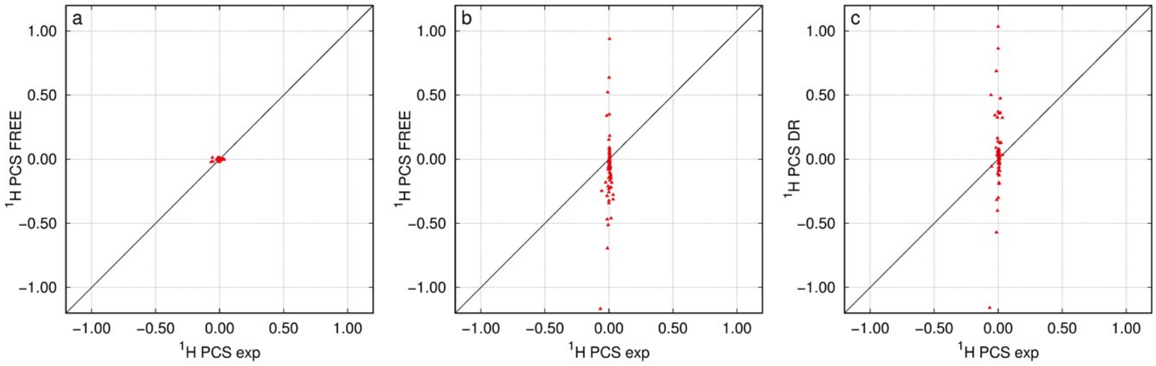

Figure S8. Correlation plots of PCS values. A) a static fit of experimental data. B) averaged PCS calculated from FREE MD trajectory. C) averaged PCS calculated from DR PCS trajectory.

Cartesian coordinates of molecular models

FeSAN optimized with PBE0 / def2-SVP (Fe: def2-TZVP)

Fe	0.0000000	0.0000000	-0.0347067
B	1.5526403	1.3222963	-0.8257376
B	1.5111003	-0.3398270	-1.4748481
B	1.5349665	1.1712046	0.9374303
C	1.5457443	-1.3351006	-0.1028660
C	1.5586669	-0.4787975	1.2456927
B	2.9981811	-1.2765135	0.8031745
B	3.0114879	0.3530933	1.4614201
B	3.0031589	-1.1608603	-0.9460123
B	3.0545312	1.4938410	0.1090056
B	3.0477333	0.5456939	-1.3910673
B	3.9620718	-0.0352314	0.0200641
H	1.1122892	2.2700785	-1.4044553
H	1.0764190	-0.7479115	-2.5020088
H	1.0340505	1.9052666	1.7369015
H	1.1088980	-2.3234685	-0.0690176
H	1.1079913	-0.9261119	2.1212836
H	3.3191217	-2.2443109	1.4104779
H	3.4194303	0.5040626	2.5684569
H	3.4128518	-2.0880324	-1.5671278
H	3.6116384	2.5424175	0.2174456
H	3.6047991	0.8947196	-2.3855515
H	5.1505546	-0.1021817	0.0546927
B	-1.5526403	-1.3222963	-0.8257376
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