Supporting Information

Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles

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Table S1: Change in RMSD (Å) and GDT-HA for the structure closest to the subset average relative to their respective values from the initial models.

Target	200 ns		8 × 3 ns	
	Δ RMSD	Δ GDT-HA	Δ RMSD	Δ GDT-HA
TR592	***-0.08***	***3.1***	***-0.03***	-0.2
TR453	0.15	-0.3	0.07	-0.3
TR432	***-0.20***	***0.4***	***-0.11***	***0.4***
TR462a	0.20	***2.7***	0.11	***0.7***
TR594	0.24	-0.2	0.04	-0.9
TR614	0.44	-1.1	0.19	-2.5
TR435	0.26	-3.8	0.08	-3.3
TR530	***-0.11***	-1.6	***-0.09***	-2.2
TR488	***-0.14***	***2.1***	***-0.07***	***0.5***
TR469	0.03	-2.8	0.00	-3.2
TR462b	0.11	***0.4***	0.08	***0.4***
TR389	***-0.21***	-5.2	0.03	-4.9
TR464	0.03	***0.7***	0.04	-0.4
TR569	***-0.30***	-1.0	***-0.03***	***0.3***
TR454	***-0.08***	***1.4***	***-0.05***	-0.1
TR567	***-0.05***	***2.6***	0.01	***2.8***
TR574	0.79	***0.7***	0.14	-2.7
TR557	***-0.50***	***1.4***	**-0.16**	***2.2***
TR429a	***-0.11***	***8.9***	0.03	***2.4***
TR517	0.31	-1.0	0.07	***0.8***
TR606	***-0.48***	***1.2***	0.02	-2.9
TR429b	***-0.13***	-0.3	***-0.06***	**0.3**
TR624	***-0.42***	***4.0***	0.06	0.0
TR568	***-0.06***	***1.6***	0.22	***0.5***
TR622	0.21	***2.5***	0.39	-0.6
TR576	0.40	-0.7	0.72	-3.3
Avg.	0.01	**0.6**	0.07	-0.6

Figure S1. Change in GDT-HA of all CASP8 and CASP9 targets after refinement without imposing restraints using C36ff

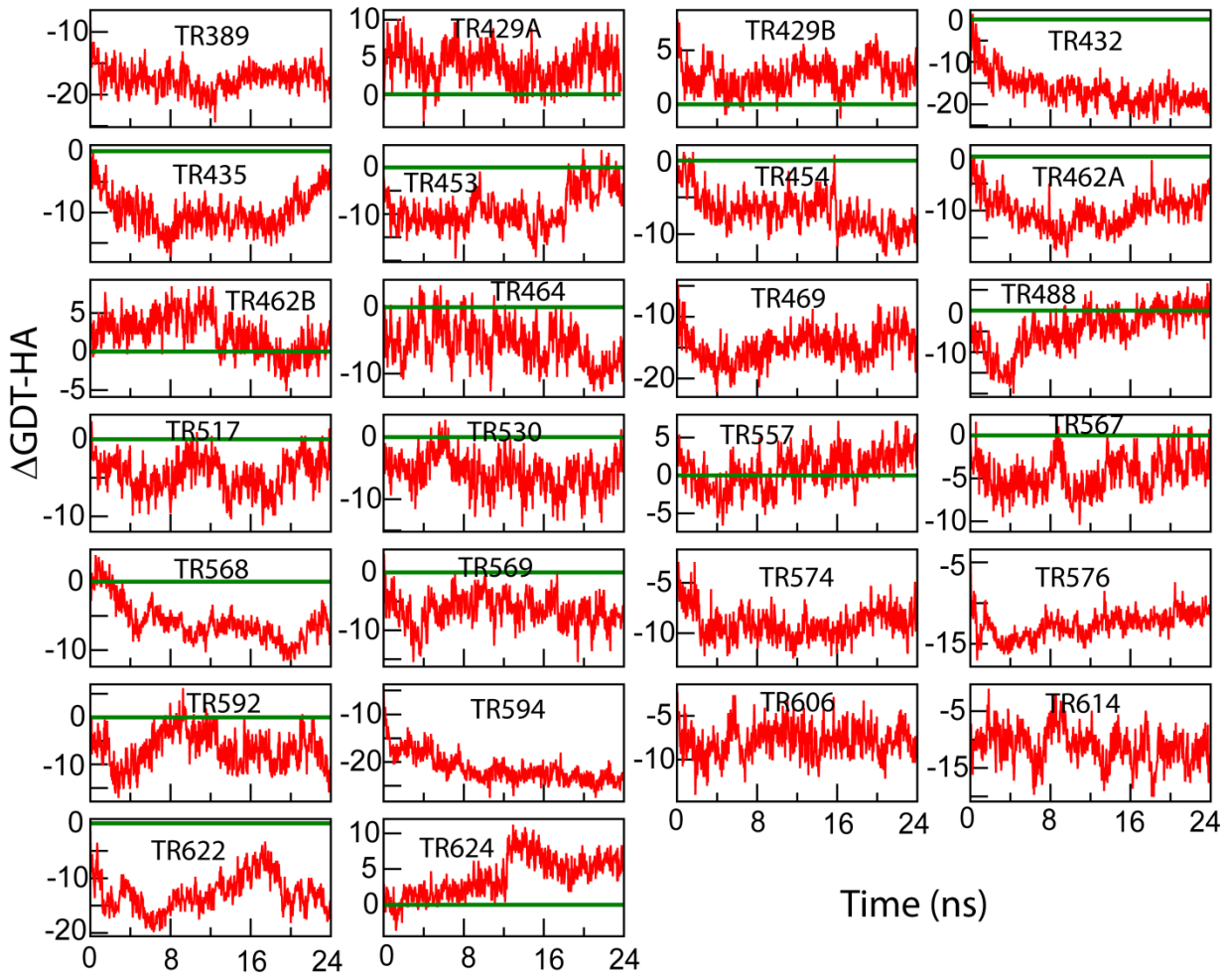

Figure S2. Change in GDT-HA vs. time for all targets with 200 ns simulation with imposed restraints