

Supporting Information

“A simple and efficient protein refinement method”

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Table S1: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_TS unit.

Table S2: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method.

Table S3: Initial GDT_HA score and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_HA unit.

Table S4: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_TS unit.

Table S5: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method.

Table S6: Initial GDT_HA score and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_HA unit.

Table S7: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory. All results are in GDT_TS unit.

Table S8: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for

CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory.

Table S9: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory. All results are in GDT_HA unit.

Table S10: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory. All results are in GDT_TS unit.

Table S11: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory.

Table S12: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory. All results are in GDT_HA unit.

Table S13: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory. All results are in GDT_TS unit.

Table S14: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory.

Table S15: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for

CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory. All results are in GDT_HA unit.

Table S16: Energy decomposition comparison for the MD0 model and Minimized-MD model for CASP10 refinement targets.

Table S17: Radius of gyration of the MD0 model and Minimized-MD model for CASP10 refinement targets.

Table S18: Model quality comparison of the starting targets, MD0 and Minimized-MD models for CASP10 refinement targets. All results are obtained by using the WHAT-CHECK program.

Table S19: Δ GDT_TS comparison between MD0 model and minimized-MD model.

Table S20: Group information for top ranked model in CASP11.

Table S21: Side chain accuracy (in terms of χ_1 and χ_2 , in percentage, using 30 degree criteria) for CASP10 starting targets, MD0 and minimized-MD model.

Table S22: Δ GDT_TS decomposition for CASP10 targets for MD0 model.

Table S1: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_TS unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	84.22	0.89	0.89	0.71	0.35	1.06	0.89	0.71	0.89	-0.71	-0.35	-0.18	0.71
TR655	78.50	-1.67	-1.17	-1.83	-0.83	-1.67	-1.50	-1.83	-0.50	-1.50	0.00	-1.33	-1.83
TR661	80.00	1.35	1.22	1.08	0.95	0.95	1.22	1.22	0.81	0.81	0.27	1.62	0.95
TR662	81.33	1.34	1.00	1.67	1.00	1.00	2.00	1.67	1.34	2.67	2.00	1.00	1.67
TR663	69.08	-0.49	-0.17	-0.33	-0.17	-0.33	-0.17	0.16	-0.33	-0.49	0.16	0.00	0.16
TR671	55.68	0.57	-0.28	0.29	0.29	0.29	0.00	0.85	0.57	-1.70	0.29	1.99	0.85
TR674	85.23	1.70	1.51	1.32	1.70	1.70	1.13	1.51	1.49	1.30	1.30	1.30	0.93
TR679	71.86	1.13	1.51	0.50	1.76	1.38	-0.25	1.38	0.38	1.00	0.50	0.75	0.88
TR681	78.27	0.79	0.26	0.79	0.00	0.26	0.39	0.66	0.51	1.14	0.89	0.89	0.00
TR688	78.38	1.48	1.48	1.35	1.48	1.76	1.76	1.48	0.94	0.81	0.67	0.81	2.03
TR689	87.80	-0.24	-0.48	-0.24	-0.24	-0.36	0.00	-0.36	-0.60	-0.48	-0.48	0.11	-0.71
TR696	70.75	0.25	-2.00	1.25	-2.25	-1.50	0.75	1.25	0.75	-1.50	-1.00	-0.50	-2.50
TR698	64.71	0.63	0.42	1.05	1.26	0.00	0.63	0.84	-0.65	0.64	0.85	-0.22	-0.43
TR699	84.11	1.22	0.78	1.11	1.11	1.33	1.22	0.67	1.11	0.67	1.33	0.78	0.67
TR704	69.70	3.78	3.14	4.22	3.24	3.46	3.89	4.00	3.35	3.03	4.22	1.30	1.40
TR705	64.58	1.57	1.83	1.31	2.35	1.57	2.09	2.09	1.83	2.61	0.00	0.26	1.57
TR708	86.48	-0.26	-0.26	-0.13	-0.38	-0.77	-0.26	-0.13	-0.38	0.13	-0.64	-0.77	-0.26
TR710	74.87	1.29	1.03	1.29	0.65	1.16	1.16	1.29	-0.51	0.13	0.26	-0.51	-0.26
TR712	92.61	0.27	0.40	0.40	0.40	0.13	-0.14	0.40	-0.14	0.00	0.13	0.54	-0.14
TR720	57.83	0.25	0.38	0.38	0.76	0.12	0.25	-0.38	-0.25	0.25	0.63	0.25	-0.38
TR722	57.09	-0.59	-0.59	-0.40	-0.40	-0.59	0.19	-0.20	-0.40	0.19	0.39	0.59	0.39
TR723	85.11	0.77	0.58	0.96	0.00	1.15	0.58	0.77	1.15	-0.76	-0.76	0.58	1.15
TR724	59.35	-0.44	-0.22	-0.44	-0.44	-0.44	0.65	-0.87	-0.22	-0.44	-1.31	-0.65	-0.22
TR738	90.06	1.71	1.41	1.41	1.71	1.10	1.21	1.21	1.00	0.40	0.70	1.51	0.80
TR747	82.50	0.56	0.28	0.00	0.00	-0.28	0.28	0.00	-0.56	-0.56	0.28	-0.83	0.28
TR750	76.79	2.61	2.61	2.06	2.74	2.88	3.02	1.78	2.88	2.19	2.47	3.16	2.47
TR752	90.37	0.17	0.00	0.00	-0.51	-0.17	-0.17	0.17	-0.84	-1.01	-1.01	-1.18	-0.34
TR754	77.94	0.37	-0.37	-0.37	0.00	-0.37	-0.73	-0.73	0.00	-0.36	-1.45	-1.09	-1.81
SUM		21.01	15.19	19.41	16.53	14.82	20.09	19.61	13.62	8.46	10.34	10.18	8.03
AVG		0.75	0.54	0.69	0.59	0.53	0.72	0.70	0.49	0.30	0.37	0.36	0.29

Table S2: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	2.712	0.008	-0.004	0.021	-0.021	0.009	0.027	0.021	-0.015	-0.018	-0.037	0.017	0.035
TR655	3.970	-0.007	-0.023	0.015	-0.032	-0.006	0.030	0.005	-0.062	-0.053	-0.028	-0.011	-0.04
TR661	2.743	-0.022	-0.008	-0.002	-0.006	0.002	-0.005	-0.007	-0.006	-0.005	0.014	-0.007	0.021
TR662	1.920	-0.022	-0.022	-0.025	-0.033	-0.010	-0.021	-0.023	-0.004	-0.008	0.004	-0.035	-0.02
TR663	3.372	0.013	0.009	0.025	-0.005	0.024	0.023	0.027	0.022	-0.009	0.001	0.010	0.029
TR671	7.716	0.092	0.100	0.085	0.123	0.086	0.079	0.095	0.108	0.151	0.042	0.067	0.056
TR674	3.444	0.055	0.061	0.041	0.040	0.083	0.046	0.035	0.113	0.064	0.050	0.075	0.148
TR679	3.949	-0.056	-0.057	-0.042	-0.046	-0.067	-0.034	-0.047	-0.018	-0.029	-0.029	-0.002	0.014
TR681	2.305	-0.043	-0.037	-0.036	-0.040	-0.024	-0.029	-0.036	0.014	0.007	-0.019	-0.047	-0.03
TR688	2.524	-0.005	-0.011	0.006	-0.012	-0.003	0.011	0.006	0.006	-0.008	-0.024	-0.023	-0.00
TR689	1.573	-0.010	-0.005	-0.010	0.010	-0.014	-0.025	0.013	0.035	0.007	0.007	-0.005	0.035
TR696	3.519	0.025	0.040	0.023	0.085	0.036	0.029	0.018	0.063	0.144	0.081	0.084	0.132
TR698	4.653	-0.020	-0.029	-0.025	-0.039	-0.012	-0.015	-0.030	0.111	0.061	0.031	0.069	0.073
TR699	2.211	-0.011	0.025	-0.036	0.036	0.018	-0.037	-0.034	0.021	-0.061	0.011	-0.040	0.030
TR704	2.540	-0.142	-0.134	-0.147	-0.128	-0.129	-0.139	-0.148	-0.147	-0.118	-0.155	-0.049	-0.03
TR705	4.709	0.031	0.060	0.009	0.072	0.043	0.024	0.000	0.015	-0.014	0.132	0.061	0.030
TR708	4.626	0.094	0.100	0.084	0.087	0.114	0.074	0.097	0.062	0.064	0.098	0.118	0.000
TR710	2.440	-0.001	-0.001	0.009	0.003	0.005	0.015	0.008	0.031	0.020	-0.018	0.039	0.040
TR712	1.992	0.014	0.025	0.004	0.034	0.018	0.013	0.004	0.051	0.044	0.045	0.043	0.031
TR720	8.515	0.058	0.066	0.051	0.062	0.063	0.051	0.060	0.055	0.045	0.064	0.093	0.032
TR722	4.422	0.044	0.043	0.039	0.042	0.044	0.033	0.054	0.009	-0.002	-0.025	-0.014	0.010
TR723	2.232	-0.022	-0.012	-0.037	0.009	-0.034	-0.046	-0.021	-0.015	0.047	0.066	0.043	-0.01
TR724	5.951	0.040	0.051	0.033	0.064	0.039	0.030	0.038	0.037	0.093	0.119	0.069	0.066
TR738	1.396	-0.109	-0.102	-0.103	-0.090	-0.097	-0.090	-0.104	-0.103	-0.083	-0.027	-0.103	-0.11
TR747	1.956	0.006	0.013	0.010	0.009	0.029	0.003	0.025	0.056	0.046	0.029	-0.029	0.057
TR750	2.125	-0.122	-0.126	-0.119	-0.128	-0.117	-0.124	-0.112	-0.096	-0.096	-0.130	-0.161	-0.12
TR752	1.495	-0.019	-0.003	-0.033	0.012	-0.016	-0.024	-0.041	-0.001	0.043	0.030	-0.018	-0.00
TR754	2.410	-0.123	-0.083	-0.144	-0.076	-0.075	-0.135	-0.135	-0.124	-0.164	-0.128	0.007	-0.13
SUM		-0.254	-0.064	-0.304	0.032	0.009	-0.236	-0.232	0.218	0.168	0.204	0.251	0.305
AVG		-0.009	-0.002	-0.011	0.001	0.000	-0.008	-0.008	0.008	0.006	0.007	0.009	0.011

Table S3: Initial GDT_HA score and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the entire 4 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_HA unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	66.84	2.66	1.95	2.66	1.25	2.66	2.84	2.31	3.90	0.36	0.89	1.42	2.49
TR655	60.33	-0.66	-0.83	-0.66	-0.16	-0.83	-0.83	-1.00	0.67	-0.83	0.00	-0.83	-1.66
TR661	59.46	2.30	1.62	1.62	1.22	1.89	1.49	1.35	1.76	1.76	1.62	2.30	1.62
TR662	60.33	2.00	1.67	2.67	2.00	1.67	3.34	2.34	2.67	4.00	3.34	1.67	2.34
TR663	49.34	-0.49	0.17	-0.66	-0.33	-0.16	-0.66	0.00	-0.49	-0.82	0.33	-0.16	0.66
TR671	36.65	0.57	0.28	0.85	0.28	1.13	0.57	1.13	1.70	-1.42	0.28	2.55	0.57
TR674	70.45	3.98	3.79	3.22	4.36	3.41	3.22	3.22	2.80	2.24	0.19	3.17	1.68
TR679	51.26	1.38	2.01	1.00	2.51	2.13	0.00	1.76	0.50	2.13	0.62	1.76	2.13
TR681	57.46	2.36	1.96	2.36	1.44	1.96	1.83	2.75	1.14	2.28	1.77	1.65	0.76
TR688	56.89	2.16	2.30	2.16	2.30	2.43	2.57	2.43	2.03	1.22	1.35	1.49	2.84
TR689	72.99	-2.02	-2.26	-2.26	-1.90	-2.49	-2.14	-2.49	-2.97	-2.14	-1.90	0.23	-3.56
TR696	50.25	0.50	-2.00	2.50	-2.75	-1.25	1.75	2.25	1.25	-1.75	-0.25	-0.25	-2.25
TR698	44.54	0.63	0.42	1.05	0.84	-0.21	1.05	0.84	-1.07	0.85	0.64	-0.64	0.00
TR699	64.44	3.12	3.12	2.23	2.45	3.23	2.78	1.89	3.56	1.45	2.89	1.45	3.12
TR704	48.48	3.90	3.14	4.66	3.47	3.68	4.23	4.44	3.47	3.47	4.55	0.76	1.20
TR705	43.75	1.82	2.08	1.56	3.39	1.56	2.60	2.60	2.08	3.13	0.52	1.04	3.13
TR708	72.19	0.39	0.39	0.90	0.26	0.13	0.64	0.77	0.26	1.41	0.13	-1.53	1.02
TR710	53.61	1.67	1.03	2.19	0.64	1.29	1.67	2.19	-0.13	0.00	0.64	0.13	0.64
TR712	80.51	1.08	0.54	1.48	0.40	0.27	0.27	0.81	-0.94	-0.67	-0.54	-0.40	0.54
TR720	39.77	0.89	1.01	1.01	1.14	0.51	0.63	-0.38	-0.12	0.63	0.89	0.38	-0.25
TR722	38.19	-0.59	-0.39	-0.20	-0.20	-0.79	0.20	0.20	-0.59	0.39	0.59	0.79	0.39
TR723	66.03	2.48	2.67	2.67	1.53	3.44	2.48	3.44	3.63	-0.38	-0.38	1.53	2.48
TR724	41.52	0.44	0.65	0.00	0.65	0.87	1.52	-0.22	1.74	0.22	-0.43	0.00	0.65
TR738	74.20	3.61	3.21	3.41	3.81	2.21	2.81	3.61	3.21	1.50	1.90	2.71	2.31
TR747	63.33	1.39	0.84	0.28	0.84	1.11	0.84	0.28	-0.55	-0.83	1.11	-0.83	0.84
TR750	55.08	3.99	3.85	3.57	3.71	4.26	4.26	3.30	4.26	3.02	3.85	3.71	3.44
TR752	75.84	-0.33	-1.18	-0.16	-1.85	-0.33	-0.16	0.00	-1.18	-2.87	-3.37	-2.87	-0.67
TR754	58.82	1.47	0.37	0.37	0.37	0.37	0.37	-0.73	1.45	-0.36	-0.72	-0.72	-2.54
SUM		40.70	32.41	40.48	31.67	34.15	40.17	39.09	34.04	17.99	20.51	20.51	23.92
AVG		1.45	1.16	1.45	1.13	1.22	1.43	1.40	1.22	0.64	0.73	0.73	0.85

Table S4: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_TS unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	84.22	0.89	0.89	0.71	0.35	1.06	0.89	0.71	0.53	0.35	-0.18	1.24	0.71
TR655	78.50	-1.67	-1.17	-1.83	-0.83	-1.67	-1.50	-1.83	-1.83	-1.33	-1.50	-1.33	-1.83
TR661	80.00	1.35	1.22	1.08	0.95	0.95	1.22	1.22	0.95	0.81	0.27	0.54	0.14
TR662	81.33	1.34	1.00	1.67	1.00	1.00	2.00	1.67	2.34	2.00	2.67	1.34	2.34
TR663	69.08	-0.49	-0.17	-0.33	-0.17	-0.33	-0.17	0.16	0.00	-0.66	0.16	-0.49	0.16
TR671	55.68	0.57	-0.28	0.29	0.29	0.29	0.00	0.85	1.14	1.99	1.42	1.99	0.85
TR674	85.23	1.70	1.51	1.32	1.70	1.70	1.13	1.51	1.30	1.11	1.67	1.49	1.49
TR679	71.86	1.13	1.51	0.50	1.76	1.38	-0.25	1.38	-0.38	1.38	0.00	-0.38	0.38
TR681	78.27	0.79	0.26	0.79	0.00	0.26	0.39	0.66	1.14	0.25	0.63	0.13	1.65
TR688	78.38	1.48	1.48	1.35	1.48	1.76	1.76	1.48	1.21	0.81	2.03	0.81	1.62
TR689	87.80	-0.24	-0.48	-0.24	-0.24	-0.36	0.00	-0.36	-0.60	-0.24	0.00	-0.71	-0.48
TR696	70.75	0.25	-2.00	1.25	-2.25	-1.50	0.75	1.25	0.50	0.75	-0.25	-0.50	0.75
TR698	64.71	0.63	0.42	1.05	1.26	0.00	0.63	0.84	0.42	0.85	-0.43	1.06	-0.43
TR699	84.11	1.22	0.78	1.11	1.11	1.33	1.22	0.67	1.22	1.11	1.00	0.89	1.67
TR704	69.70	3.78	3.14	4.22	3.24	3.46	3.89	4.00	3.89	4.22	3.14	2.70	3.14
TR705	64.58	1.57	1.83	1.31	2.35	1.57	2.09	2.09	1.31	1.31	1.57	0.52	1.05
TR708	86.48	-0.26	-0.26	-0.13	-0.38	-0.77	-0.26	-0.13	-0.13	-1.02	-0.51	-0.51	-0.26
TR710	74.87	1.29	1.03	1.29	0.65	1.16	1.16	1.29	0.13	0.39	0.00	-0.26	-0.51
TR712	92.61	0.27	0.40	0.40	0.40	0.13	-0.14	0.40	-0.41	0.67	0.13	-0.41	-0.14
TR720	57.83	0.25	0.38	0.38	0.76	0.12	0.25	-0.38	-0.38	-0.51	0.12	0.12	-0.38
TR722	57.09	-0.59	-0.59	-0.40	-0.40	-0.59	0.19	-0.20	0.39	0.19	0.19	0.59	0.39
TR723	85.11	0.77	0.58	0.96	0.00	1.15	0.58	0.77	1.34	1.15	0.96	1.34	1.15
TR724	59.35	-0.44	-0.22	-0.44	-0.44	-0.44	0.65	-0.87	-0.22	-0.44	-1.31	-0.44	0.00
TR738	90.06	1.71	1.41	1.41	1.71	1.10	1.21	1.21	1.10	0.90	0.10	1.31	1.00
TR747	82.50	0.56	0.28	0.00	0.00	-0.28	0.28	0.00	0.28	0.28	-0.28	-0.83	0.28
TR750	76.79	2.61	2.61	2.06	2.74	2.88	3.02	1.78	1.92	2.47	2.61	2.19	2.47
TR752	90.37	0.17	0.00	0.00	-0.51	-0.17	-0.17	0.17	-0.84	-0.51	-0.17	-1.01	-0.17
TR754	77.94	0.37	-0.37	-0.37	0.00	-0.37	-0.73	-0.73	-0.36	-0.36	0.36	-0.36	-0.72
SUM		21.01	15.19	19.41	16.53	14.82	20.09	19.61	15.96	17.92	14.40	11.03	16.32
AVG		0.75	0.54	0.69	0.59	0.53	0.72	0.70	0.57	0.64	0.51	0.39	0.58

Table S5: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	2.712	0.008	-0.004	0.021	-0.021	0.009	0.027	0.021	0.019	0.039	0.017	-0.017	0.035
TR655	3.970	-0.007	-0.023	0.015	-0.032	-0.006	0.030	0.005	-0.039	-0.011	0.034	-0.033	-0.042
TR661	2.743	-0.022	-0.008	-0.002	-0.006	0.002	-0.005	-0.007	0.006	0.004	0.013	-0.014	0.010
TR662	1.920	-0.022	-0.022	-0.025	-0.033	-0.010	-0.021	-0.023	-0.045	-0.020	-0.008	-0.018	-0.059
TR663	3.372	0.013	0.009	0.025	-0.005	0.024	0.023	0.027	0.017	0.055	0.029	0.035	0.025
TR671	7.716	0.092	0.100	0.085	0.123	0.086	0.079	0.095	0.102	0.109	0.010	0.067	0.056
TR674	3.444	0.055	0.061	0.041	0.040	0.083	0.046	0.035	0.070	0.051	0.052	0.061	0.058
TR679	3.949	-0.056	-0.057	-0.042	-0.046	-0.067	-0.034	-0.047	-0.009	-0.033	-0.005	-0.015	-0.034
TR681	2.305	-0.043	-0.037	-0.036	-0.040	-0.024	-0.029	-0.036	-0.011	-0.003	-0.001	0.018	0.011
TR688	2.524	-0.005	-0.011	0.006	-0.012	-0.003	0.011	0.006	0.008	0.022	-0.033	0.057	0.008
TR689	1.573	-0.010	-0.005	-0.010	0.010	-0.014	-0.025	0.013	0.028	-0.017	-0.021	0.035	0.015
TR696	3.519	0.025	0.040	0.023	0.085	0.036	0.029	0.018	0.055	0.036	0.059	0.075	0.084
TR698	4.653	-0.020	-0.029	-0.025	-0.039	-0.012	-0.015	-0.030	0.048	0.031	0.038	0.037	0.073
TR699	2.211	-0.011	0.025	-0.036	0.036	0.018	-0.037	-0.034	-0.063	-0.042	-0.044	-0.005	-0.058
TR704	2.540	-0.142	-0.134	-0.147	-0.128	-0.129	-0.139	-0.148	-0.152	-0.184	-0.122	-0.133	-0.123
TR705	4.709	0.031	0.060	0.009	0.072	0.043	0.024	0.000	0.011	-0.009	0.053	0.061	-0.010
TR708	4.626	0.094	0.100	0.084	0.087	0.114	0.074	0.097	0.068	0.072	0.075	0.069	0.000
TR710	2.440	-0.001	-0.001	0.009	0.003	0.005	0.015	0.008	0.031	-0.002	0.036	0.040	0.025
TR712	1.992	0.014	0.025	0.004	0.034	0.018	0.013	0.004	0.018	0.007	0.039	0.036	0.031
TR720	8.515	0.058	0.066	0.051	0.062	0.063	0.051	0.060	0.060	0.050	0.081	0.044	0.032
TR722	4.422	0.044	0.043	0.039	0.042	0.044	0.033	0.054	0.008	-0.021	0.000	-0.014	0.010
TR723	2.232	-0.022	-0.012	-0.037	0.009	-0.034	-0.046	-0.021	-0.019	-0.025	0.037	-0.029	-0.013
TR724	5.951	0.040	0.051	0.033	0.064	0.039	0.030	0.038	0.051	0.050	0.119	0.074	0.033
TR738	1.396	-0.109	-0.102	-0.103	-0.090	-0.097	-0.090	-0.104	-0.116	-0.083	-0.081	-0.086	-0.101
TR747	1.956	0.006	0.013	0.010	0.009	0.029	0.003	0.025	0.042	0.029	0.057	-0.029	0.057
TR750	2.125	-0.122	-0.126	-0.119	-0.128	-0.117	-0.124	-0.112	-0.102	-0.102	-0.116	-0.101	-0.129
TR752	1.495	-0.019	-0.003	-0.033	0.012	-0.016	-0.024	-0.041	0.009	0.005	-0.040	0.021	-0.016
TR754	2.410	-0.123	-0.083	-0.144	-0.076	-0.075	-0.135	-0.135	-0.164	-0.126	-0.153	-0.157	-0.103
SUM		-0.254	-0.064	-0.304	0.032	0.009	-0.236	-0.232	-0.069	-0.118	0.125	0.079	-0.125
AVG		-0.009	-0.002	-0.011	0.001	0.000	-0.008	-0.008	-0.002	-0.004	0.004	0.003	-0.004

Table S6: Initial GDT_HA score and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our clustering model selection results. We used the last 2 ns production trajectory with AMBER RMSD clustering method. All results are in GDT_HA unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	Cluster1	Cluster2	Cluster3	Cluster4	Cluster5
TR644	66.84	2.66	1.95	2.66	1.25	2.66	2.84	2.31	3.02	2.49	1.42	3.55	2.49
TR655	60.33	-0.66	-0.83	-0.66	-0.16	-0.83	-0.83	-1.00	-0.83	-0.83	-0.33	0.00	-1.66
TR661	59.46	2.30	1.62	1.62	1.22	1.89	1.49	1.35	2.43	1.49	1.08	0.95	1.08
TR662	60.33	2.00	1.67	2.67	2.00	1.67	3.34	2.34	3.67	2.67	4.00	2.34	4.00
TR663	49.34	-0.49	0.17	-0.66	-0.33	-0.16	-0.66	0.00	-0.16	-0.82	0.66	-0.49	-0.33
TR671	36.65	0.57	0.28	0.85	0.28	1.13	0.57	1.13	1.42	2.27	1.70	2.55	0.57
TR674	70.45	3.98	3.79	3.22	4.36	3.41	3.22	3.22	2.61	0.19	3.73	0.94	1.31
TR679	51.26	1.38	2.01	1.00	2.51	2.13	0.00	1.76	-0.13	2.13	0.37	0.00	0.50
TR681	57.46	2.36	1.96	2.36	1.44	1.96	1.83	2.75	2.03	0.76	1.39	0.89	2.54
TR688	56.89	2.16	2.30	2.16	2.30	2.43	2.57	2.43	1.49	1.49	2.70	1.49	2.30
TR689	72.99	-2.02	-2.26	-2.26	-1.90	-2.49	-2.14	-2.49	-2.73	-1.54	-2.02	-3.56	-1.07
TR696	50.25	0.50	-2.00	2.50	-2.75	-1.25	1.75	2.25	1.00	0.75	0.00	-0.25	1.25
TR698	44.54	0.63	0.42	1.05	0.84	-0.21	1.05	0.84	1.28	0.64	0.21	2.14	0.00
TR699	64.44	3.12	3.12	2.23	2.45	3.23	2.78	1.89	3.12	2.56	1.56	2.34	3.23
TR704	48.48	3.90	3.14	4.66	3.47	3.68	4.23	4.44	4.33	4.44	3.14	2.93	3.25
TR705	43.75	1.82	2.08	1.56	3.39	1.56	2.60	2.60	2.08	1.82	2.60	1.30	1.82
TR708	72.19	0.39	0.39	0.90	0.26	0.13	0.64	0.77	0.90	-0.63	0.39	-0.25	1.02
TR710	53.61	1.67	1.03	2.19	0.64	1.29	1.67	2.19	0.90	1.42	0.64	0.64	0.00
TR712	80.51	1.08	0.54	1.48	0.40	0.27	0.27	0.81	-0.40	0.81	0.14	0.14	0.54
TR720	39.77	0.89	1.01	1.01	1.14	0.51	0.63	-0.38	-0.25	-0.25	0.63	0.63	-0.25
TR722	38.19	-0.59	-0.39	-0.20	-0.20	-0.79	0.20	0.20	0.79	0.00	0.39	0.79	0.39
TR723	66.03	2.48	2.67	2.67	1.53	3.44	2.48	3.44	2.48	3.24	4.01	1.91	2.48
TR724	41.52	0.44	0.65	0.00	0.65	0.87	1.52	-0.22	1.09	0.44	-0.43	1.09	1.31
TR738	74.20	3.61	3.21	3.41	3.81	2.21	2.81	3.61	3.21	2.41	1.50	3.41	2.61
TR747	63.33	1.39	0.84	0.28	0.84	1.11	0.84	0.28	0.28	1.11	0.00	-0.83	0.84
TR750	55.08	3.99	3.85	3.57	3.71	4.26	4.26	3.30	3.16	3.02	3.85	3.16	3.44
TR752	75.84	-0.33	-1.18	-0.16	-1.85	-0.33	-0.16	0.00	-1.01	-0.67	0.85	-1.35	-0.33
TR754	58.82	1.47	0.37	0.37	0.37	0.37	0.37	-0.73	-0.36	0.00	1.09	0.36	0.73
SUM		40.70	32.41	40.48	31.67	34.15	40.17	39.09	35.42	31.41	35.27	26.82	34.06
AVG		1.45	1.16	1.45	1.13	1.22	1.43	1.40	1.27	1.12	1.26	0.96	1.22

Table S7: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory. All results are in GDT_TS unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	20% of 4ns	40% of 2ns
TR644	84.22	0.89	0.89	0.71	0.35	1.06	0.89	0.71	0.18	-1.06
TR655	78.50	-1.67	-1.17	-1.83	-0.83	-1.67	-1.50	-1.83	0.33	1.67
TR661	80.00	1.35	1.22	1.08	0.95	0.95	1.22	1.22	0.68	1.08
TR662	81.33	1.34	1.00	1.67	1.00	1.00	2.00	1.67	1.67	-0.33
TR663	69.08	-0.49	-0.17	-0.33	-0.17	-0.33	-0.17	0.16	0.33	-0.33
TR671	55.68	0.57	-0.28	0.29	0.29	0.29	0.00	0.85	-0.85	3.13
TR674	85.23	1.70	1.51	1.32	1.70	1.70	1.13	1.51	0.78	0.96
TR679	71.86	1.13	1.51	0.50	1.76	1.38	-0.25	1.38	0.25	0.25
TR681	78.27	0.79	0.26	0.79	0.00	0.26	0.39	0.66	-2.13	-0.22
TR688	78.38	1.48	1.48	1.35	1.48	1.76	1.76	1.48	0.27	1.48
TR689	87.80	-0.24	-0.48	-0.24	-0.24	-0.36	0.00	-0.36	0.00	-0.12
TR696	70.75	0.25	-2.00	1.25	-2.25	-1.50	0.75	1.25	-2.00	2.00
TR698	64.71	0.63	0.42	1.05	1.26	0.00	0.63	0.84	1.53	1.10
TR699	84.11	1.22	0.78	1.11	1.11	1.33	1.22	0.67	-0.89	-0.22
TR704	69.70	3.78	3.14	4.22	3.24	3.46	3.89	4.00	2.38	3.57
TR705	64.58	1.57	1.83	1.31	2.35	1.57	2.09	2.09	1.83	4.43
TR708	86.48	-0.26	-0.26	-0.13	-0.38	-0.77	-0.26	-0.13	-1.28	-1.53
TR710	74.87	1.29	1.03	1.29	0.65	1.16	1.16	1.29	0.65	-0.64
TR712	92.61	0.27	0.40	0.40	0.40	0.13	-0.14	0.40	0.13	0.80
TR720	57.83	0.25	0.38	0.38	0.76	0.12	0.25	-0.38	0.38	0.63
TR722	57.09	-0.59	-0.59	-0.40	-0.40	-0.59	0.19	-0.20	0.59	0.39
TR723	85.11	0.77	0.58	0.96	0.00	1.15	0.58	0.77	-1.71	1.91
TR724	59.35	-0.44	-0.22	-0.44	-0.44	-0.44	0.65	-0.87	-0.65	-0.22
TR738	90.06	1.71	1.41	1.41	1.71	1.10	1.21	1.21	0.40	2.21
TR747	82.50	0.56	0.28	0.00	0.00	-0.28	0.28	0.00	-0.83	-1.94
TR750	76.79	2.61	2.61	2.06	2.74	2.88	3.02	1.78	2.19	2.06
TR752	90.37	0.17	0.00	0.00	-0.51	-0.17	-0.17	0.17	-0.84	-1.18
TR754	77.94	0.37	-0.37	-0.37	0.00	-0.37	-0.73	-0.73	-4.03	-5.48
SUM		21.01	15.19	19.41	16.53	14.82	20.09	19.61	-0.64	14.40
AVG		0.75	0.54	0.69	0.59	0.53	0.72	0.70	-0.02	0.51

Table S8: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	20% of 4ns	40% of 2ns
TR644	2.712	0.008	-0.004	0.021	-0.021	0.009	0.027	0.021	-0.012	-0.091
TR655	3.970	-0.007	-0.023	0.015	-0.032	-0.006	0.030	0.005	-0.096	-0.165
TR661	2.743	-0.022	-0.008	-0.002	-0.006	0.002	-0.005	-0.007	0.025	0.016
TR662	1.920	-0.022	-0.022	-0.025	-0.033	-0.010	-0.021	-0.023	-0.040	0.028
TR663	3.372	0.013	0.009	0.025	-0.005	0.024	0.023	0.027	-0.045	-0.013
TR671	7.716	0.092	0.100	0.085	0.123	0.086	0.079	0.095	0.113	-0.067
TR674	3.444	0.055	0.061	0.041	0.040	0.083	0.046	0.035	0.049	0.118
TR679	3.949	-0.056	-0.057	-0.042	-0.046	-0.067	-0.034	-0.047	0.044	0.017
TR681	2.305	-0.043	-0.037	-0.036	-0.040	-0.024	-0.029	-0.036	0.337	0.376
TR688	2.524	-0.005	-0.011	0.006	-0.012	-0.003	0.011	0.006	0.012	0.050
TR689	1.573	-0.010	-0.005	-0.010	0.010	-0.014	-0.025	0.013	0.009	-0.025
TR696	3.519	0.025	0.040	0.023	0.085	0.036	0.029	0.018	0.057	-0.038
TR698	4.653	-0.020	-0.029	-0.025	-0.039	-0.012	-0.015	-0.030	-0.621	-0.676
TR699	2.211	-0.011	0.025	-0.036	0.036	0.018	-0.037	-0.034	0.038	-0.037
TR704	2.540	-0.142	-0.134	-0.147	-0.128	-0.129	-0.139	-0.148	-0.051	-0.113
TR705	4.709	0.031	0.060	0.009	0.072	0.043	0.024	0.000	0.112	-0.019
TR708	4.626	0.094	0.100	0.084	0.087	0.114	0.074	0.097	0.089	0.112
TR710	2.440	-0.001	-0.001	0.009	0.003	0.005	0.015	0.008	-0.050	0.042
TR712	1.992	0.014	0.025	0.004	0.034	0.018	0.013	0.004	0.022	-0.011
TR720	8.515	0.058	0.066	0.051	0.062	0.063	0.051	0.060	0.092	0.246
TR722	4.422	0.044	0.043	0.039	0.042	0.044	0.033	0.054	-0.007	0.066
TR723	2.232	-0.022	-0.012	-0.037	0.009	-0.034	-0.046	-0.021	0.065	0.002
TR724	5.951	0.040	0.051	0.033	0.064	0.039	0.030	0.038	0.116	0.087
TR738	1.396	-0.109	-0.102	-0.103	-0.090	-0.097	-0.090	-0.104	-0.039	-0.170
TR747	1.956	0.006	0.013	0.010	0.009	0.029	0.003	0.025	0.043	0.134
TR750	2.125	-0.122	-0.126	-0.119	-0.128	-0.117	-0.124	-0.112	-0.091	-0.126
TR752	1.495	-0.019	-0.003	-0.033	0.012	-0.016	-0.024	-0.041	0.047	0.017
TR754	2.410	-0.123	-0.083	-0.144	-0.076	-0.075	-0.135	-0.135	0.039	0.036
SUM		-0.254	-0.064	-0.304	0.032	0.009	-0.236	-0.232	0.257	-0.204
AVG		-0.009	-0.002	-0.011	0.001	0.000	-0.008	-0.008	0.009	-0.007

Table S9: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We used ProQ2 program to select 20% of the top ranked structures from the entire 4 ns trajectory and 40% of the last 2 ns trajectory. All results are in GDT_HA unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	20% of 4ns	40% of 2ns
TR644	66.84	2.66	1.95	2.66	1.25	2.66	2.84	2.31	1.60	0.18
TR655	60.33	-0.66	-0.83	-0.66	-0.16	-0.83	-0.83	-1.00	1.67	2.00
TR661	59.46	2.30	1.62	1.62	1.22	1.89	1.49	1.35	1.49	2.03
TR662	60.33	2.00	1.67	2.67	2.00	1.67	3.34	2.34	2.34	0.34
TR663	49.34	-0.49	0.17	-0.66	-0.33	-0.16	-0.66	0.00	0.33	-0.82
TR671	36.65	0.57	0.28	0.85	0.28	1.13	0.57	1.13	-0.85	3.12
TR674	70.45	3.98	3.79	3.22	4.36	3.41	3.22	3.22	3.62	4.55
TR679	51.26	1.38	2.01	1.00	2.51	2.13	0.00	1.76	0.25	0.62
TR681	57.46	2.36	1.96	2.36	1.44	1.96	1.83	2.75	-1.75	1.04
TR688	56.89	2.16	2.30	2.16	2.30	2.43	2.57	2.43	0.27	1.76
TR689	72.99	-2.02	-2.26	-2.26	-1.90	-2.49	-2.14	-2.49	-0.95	-2.14
TR696	50.25	0.50	-2.00	2.50	-2.75	-1.25	1.75	2.25	-2.50	3.00
TR698	44.54	0.63	0.42	1.05	0.84	-0.21	1.05	0.84	0.76	0.97
TR699	64.44	3.12	3.12	2.23	2.45	3.23	2.78	1.89	0.23	0.67
TR704	48.48	3.90	3.14	4.66	3.47	3.68	4.23	4.44	2.39	3.90
TR705	43.75	1.82	2.08	1.56	3.39	1.56	2.60	2.60	1.56	7.81
TR708	72.19	0.39	0.39	0.90	0.26	0.13	0.64	0.77	-1.40	-0.51
TR710	53.61	1.67	1.03	2.19	0.64	1.29	1.67	2.19	1.03	0.00
TR712	80.51	1.08	0.54	1.48	0.40	0.27	0.27	0.81	-0.67	-0.81
TR720	39.77	0.89	1.01	1.01	1.14	0.51	0.63	-0.38	0.63	0.89
TR722	38.19	-0.59	-0.39	-0.20	-0.20	-0.79	0.20	0.20	0.79	0.59
TR723	66.03	2.48	2.67	2.67	1.53	3.44	2.48	3.44	-1.14	2.86
TR724	41.52	0.44	0.65	0.00	0.65	0.87	1.52	-0.22	-0.87	0.22
TR738	74.20	3.61	3.21	3.41	3.81	2.21	2.81	3.61	1.00	3.61
TR747	63.33	1.39	0.84	0.28	0.84	1.11	0.84	0.28	-0.83	-2.50
TR750	55.08	3.99	3.85	3.57	3.71	4.26	4.26	3.30	3.85	4.67
TR752	75.84	-0.33	-1.18	-0.16	-1.85	-0.33	-0.16	0.00	-2.36	-2.70
TR754	58.82	1.47	0.37	0.37	0.37	0.37	0.37	-0.73	-3.39	-6.65
SUM		40.70	32.41	40.48	31.67	34.15	40.17	39.09	7.10	28.70
AVG		1.45	1.16	1.45	1.13	1.22	1.43	1.40	0.25	1.03

Table S10: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory. All results are in GDT_TS unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	84.22	0.89	0.89	0.71	0.35	1.06	0.89	0.71	-1.60	-1.77	-1.60
TR655	78.50	-1.67	-1.17	-1.83	-0.83	-1.67	-1.50	-1.83	0.67	0.83	0.17
TR661	80.00	1.35	1.22	1.08	0.95	0.95	1.22	1.22	-0.14	0.27	-0.68
TR662	81.33	1.34	1.00	1.67	1.00	1.00	2.00	1.67	0.00	0.67	1.67
TR663	69.08	-0.49	-0.17	-0.33	-0.17	-0.33	-0.17	0.16	0.16	0.16	0.49
TR671	55.68	0.57	-0.28	0.29	0.29	0.29	0.00	0.85	1.14	0.85	1.14
TR674	85.23	1.70	1.51	1.32	1.70	1.70	1.13	1.51	-0.16	0.03	-0.72
TR679	71.86	1.13	1.51	0.50	1.76	1.38	-0.25	1.38	1.26	1.13	0.38
TR681	78.27	0.79	0.26	0.79	0.00	0.26	0.39	0.66	-2.38	-2.25	-2.51
TR688	78.38	1.48	1.48	1.35	1.48	1.76	1.76	1.48	2.97	1.62	2.03
TR689	87.80	-0.24	-0.48	-0.24	-0.24	-0.36	0.00	-0.36	-0.95	-1.43	-0.83
TR696	70.75	0.25	-2.00	1.25	-2.25	-1.50	0.75	1.25	1.75	1.75	1.75
TR698	64.71	0.63	0.42	1.05	1.26	0.00	0.63	0.84	1.53	0.67	0.67
TR699	84.11	1.22	0.78	1.11	1.11	1.33	1.22	0.67	-1.22	-1.44	-1.00
TR704	69.70	3.78	3.14	4.22	3.24	3.46	3.89	4.00	4.87	4.98	4.00
TR705	64.58	1.57	1.83	1.31	2.35	1.57	2.09	2.09	4.69	4.17	3.39
TR708	86.48	-0.26	-0.26	-0.13	-0.38	-0.77	-0.26	-0.13	-0.89	-0.64	-0.26
TR710	74.87	1.29	1.03	1.29	0.65	1.16	1.16	1.29	0.77	0.90	0.65
TR712	92.61	0.27	0.40	0.40	0.40	0.13	-0.14	0.40	0.80	1.07	0.40
TR720	57.83	0.25	0.38	0.38	0.76	0.12	0.25	-0.38	0.38	0.50	0.12
TR722	57.09	-0.59	-0.59	-0.40	-0.40	-0.59	0.19	-0.20	0.00	0.00	-0.59
TR723	85.11	0.77	0.58	0.96	0.00	1.15	0.58	0.77	0.96	1.15	1.53
TR724	59.35	-0.44	-0.22	-0.44	-0.44	-0.44	0.65	-0.87	-0.87	-1.52	-1.09
TR738	90.06	1.71	1.41	1.41	1.71	1.10	1.21	1.21	2.11	2.11	2.51
TR747	82.50	0.56	0.28	0.00	0.00	-0.28	0.28	0.00	-1.11	-1.11	-0.28
TR750	76.79	2.61	2.61	2.06	2.74	2.88	3.02	1.78	2.74	2.61	2.61
TR752	90.37	0.17	0.00	0.00	-0.51	-0.17	-0.17	0.17	-0.84	-0.51	-0.51
TR754	77.94	0.37	-0.37	-0.37	0.00	-0.37	-0.73	-0.73	-8.37	-7.65	-6.56
SUM		21.01	15.19	19.41	16.53	14.82	20.09	19.61	8.270	7.150	6.880
AVG		0.75	0.54	0.69	0.59	0.53	0.72	0.70	0.295	0.255	0.246

Table S11: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	2.712	0.008	-0.004	0.021	-0.021	0.009	0.027	0.021	-0.077	-0.117	-0.083
TR655	3.970	-0.007	-0.023	0.015	-0.032	-0.006	0.030	0.005	-0.163	-0.161	-0.138
TR661	2.743	-0.022	-0.008	-0.002	-0.006	0.002	-0.005	-0.007	-0.031	-0.013	0.010
TR662	1.920	-0.022	-0.022	-0.025	-0.033	-0.010	-0.021	-0.023	0.038	0.005	-0.020
TR663	3.372	0.013	0.009	0.025	-0.005	0.024	0.023	0.027	-0.017	-0.057	-0.009
TR671	7.716	0.092	0.100	0.085	0.123	0.086	0.079	0.095	-0.026	-0.037	0.043
TR674	3.444	0.055	0.061	0.041	0.040	0.083	0.046	0.035	0.142	0.141	0.149
TR679	3.949	-0.056	-0.057	-0.042	-0.046	-0.067	-0.034	-0.047	0.011	-0.006	0.038
TR681	2.305	-0.043	-0.037	-0.036	-0.040	-0.024	-0.029	-0.036	0.391	0.390	0.394
TR688	2.524	-0.005	-0.011	0.006	-0.012	-0.003	0.011	0.006	0.016	0.023	0.028
TR689	1.573	-0.010	-0.005	-0.010	0.010	-0.014	-0.025	0.013	0.034	0.050	0.058
TR696	3.519	0.025	0.040	0.023	0.085	0.036	0.029	0.018	-0.040	-0.029	-0.039
TR698	4.653	-0.020	-0.029	-0.025	-0.039	-0.012	-0.015	-0.030	-0.685	-0.679	-0.685
TR699	2.211	-0.011	0.025	-0.036	0.036	0.018	-0.037	-0.034	0.024	0.026	0.033
TR704	2.540	-0.142	-0.134	-0.147	-0.128	-0.129	-0.139	-0.148	-0.196	-0.148	-0.107
TR705	4.709	0.031	0.060	0.009	0.072	0.043	0.024	0.000	-0.089	-0.070	-0.099
TR708	4.626	0.094	0.100	0.084	0.087	0.114	0.074	0.097	0.133	0.081	0.025
TR710	2.440	-0.001	-0.001	0.009	0.003	0.005	0.015	0.008	-0.041	-0.039	-0.011
TR712	1.992	0.014	0.025	0.004	0.034	0.018	0.013	0.004	0.013	0.009	0.028
TR720	8.515	0.058	0.066	0.051	0.062	0.063	0.051	0.060	0.235	0.243	0.224
TR722	4.422	0.044	0.043	0.039	0.042	0.044	0.033	0.054	0.070	0.081	0.073
TR723	2.232	-0.022	-0.012	-0.037	0.009	-0.034	-0.046	-0.021	0.053	0.053	0.063
TR724	5.951	0.040	0.051	0.033	0.064	0.039	0.030	0.038	0.008	0.016	0.010
TR738	1.396	-0.109	-0.102	-0.103	-0.090	-0.097	-0.090	-0.104	-0.184	-0.199	-0.216
TR747	1.956	0.006	0.013	0.010	0.009	0.029	0.003	0.025	0.094	0.082	0.099
TR750	2.125	-0.122	-0.126	-0.119	-0.128	-0.117	-0.124	-0.112	-0.127	-0.131	-0.131
TR752	1.495	-0.019	-0.003	-0.033	0.012	-0.016	-0.024	-0.041	-0.001	-0.035	-0.038
TR754	2.410	-0.123	-0.083	-0.144	-0.076	-0.075	-0.135	-0.135	0.121	0.117	0.011
SUM		-0.254	-0.064	-0.304	0.032	0.009	-0.236	-0.232	-0.294	-0.404	-0.290
AVG		-0.009	-0.002	-0.011	0.001	0.000	-0.008	-0.008	-0.011	-0.014	-0.010

Table S12: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low AMBER energy plus DFIRE energy ($E_{AMBER}+E_{DFIRE}$) structures from the last 2 ns trajectory. All results are in GDT_HA unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	66.84	2.66	1.95	2.66	1.25	2.66	2.84	2.31	0.18	-0.17	0.36
TR655	60.33	-0.66	-0.83	-0.66	-0.16	-0.83	-0.83	-1.00	0.34	0.84	1.00
TR661	59.46	2.30	1.62	1.62	1.22	1.89	1.49	1.35	1.08	1.22	0.27
TR662	60.33	2.00	1.67	2.67	2.00	1.67	3.34	2.34	0.34	1.34	2.34
TR663	49.34	-0.49	0.17	-0.66	-0.33	-0.16	-0.66	0.00	-0.16	-0.33	0.17
TR671	36.65	0.57	0.28	0.85	0.28	1.13	0.57	1.13	1.13	1.13	1.42
TR674	70.45	3.98	3.79	3.22	4.36	3.41	3.22	3.22	2.68	3.06	1.38
TR679	51.26	1.38	2.01	1.00	2.51	2.13	0.00	1.76	2.26	2.01	0.88
TR681	57.46	2.36	1.96	2.36	1.44	1.96	1.83	2.75	-1.11	-1.24	-1.88
TR688	56.89	2.16	2.30	2.16	2.30	2.43	2.57	2.43	3.38	2.30	2.57
TR689	72.99	-2.02	-2.26	-2.26	-1.90	-2.49	-2.14	-2.49	-4.15	-4.63	-3.44
TR696	50.25	0.50	-2.00	2.50	-2.75	-1.25	1.75	2.25	2.50	3.25	3.00
TR698	44.54	0.63	0.42	1.05	0.84	-0.21	1.05	0.84	1.61	0.76	0.97
TR699	64.44	3.12	3.12	2.23	2.45	3.23	2.78	1.89	-0.44	-0.44	-0.11
TR704	48.48	3.90	3.14	4.66	3.47	3.68	4.23	4.44	5.63	5.74	4.33
TR705	43.75	1.82	2.08	1.56	3.39	1.56	2.60	2.60	6.77	6.25	5.47
TR708	72.19	0.39	0.39	0.90	0.26	0.13	0.64	0.77	-1.14	-1.14	0.13
TR710	53.61	1.67	1.03	2.19	0.64	1.29	1.67	2.19	2.58	2.83	2.45
TR712	80.51	1.08	0.54	1.48	0.40	0.27	0.27	0.81	0.00	1.08	-0.67
TR720	39.77	0.89	1.01	1.01	1.14	0.51	0.63	-0.38	0.76	1.39	0.51
TR722	38.19	-0.59	-0.39	-0.20	-0.20	-0.79	0.20	0.20	-0.20	-0.20	-0.39
TR723	66.03	2.48	2.67	2.67	1.53	3.44	2.48	3.44	1.91	1.91	2.10
TR724	41.52	0.44	0.65	0.00	0.65	0.87	1.52	-0.22	-0.87	-1.74	-1.30
TR738	74.20	3.61	3.21	3.41	3.81	2.21	2.81	3.61	4.41	3.71	4.01
TR747	63.33	1.39	0.84	0.28	0.84	1.11	0.84	0.28	-1.66	-0.83	0.84
TR750	55.08	3.99	3.85	3.57	3.71	4.26	4.26	3.30	6.05	5.77	5.63
TR752	75.84	-0.33	-1.18	-0.16	-1.85	-0.33	-0.16	0.00	-2.19	-1.68	-2.02
TR754	58.82	1.47	0.37	0.37	0.37	0.37	0.37	-0.73	-9.91	-9.18	-7.73
SUM		40.70	32.41	40.48	31.67	34.15	40.17	39.09	21.780	23.010	22.29
AVG		1.45	1.16	1.45	1.13	1.22	1.43	1.40	0.778	0.822	0.796

Table S13: Initial GDT_TS scores, and Δ GDT_TS results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory. All results are in GDT_TS unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	84.22	0.89	0.89	0.71	0.35	1.06	0.89	0.71	-1.24	-0.89	-1.95
TR655	78.50	-1.67	-1.17	-1.83	-0.83	-1.67	-1.50	-1.83	0.17	0.83	0.67
TR661	80.00	1.35	1.22	1.08	0.95	0.95	1.22	1.22	-0.95	0.27	-1.08
TR662	81.33	1.34	1.00	1.67	1.00	1.00	2.00	1.67	0.00	0.00	1.34
TR663	69.08	-0.49	-0.17	-0.33	-0.17	-0.33	-0.17	0.16	0.49	0.16	0.16
TR671	55.68	0.57	-0.28	0.29	0.29	0.29	0.00	0.85	0.85	0.85	1.42
TR674	85.23	1.70	1.51	1.32	1.70	1.70	1.13	1.51	-0.16	-1.09	-0.72
TR679	71.86	1.13	1.51	0.50	1.76	1.38	-0.25	1.38	1.13	0.88	1.00
TR681	78.27	0.79	0.26	0.79	0.00	0.26	0.39	0.66	-2.51	-2.13	-1.87
TR688	78.38	1.48	1.48	1.35	1.48	1.76	1.76	1.48	2.97	2.43	2.70
TR689	87.80	-0.24	-0.48	-0.24	-0.24	-0.36	0.00	-0.36	-1.07	-1.31	-0.48
TR696	70.75	0.25	-2.00	1.25	-2.25	-1.50	0.75	1.25	1.75	1.50	2.00
TR698	64.71	0.63	0.42	1.05	1.26	0.00	0.63	0.84	1.32	1.53	1.10
TR699	84.11	1.22	0.78	1.11	1.11	1.33	1.22	0.67	-1.33	-1.22	-0.78
TR704	69.70	3.78	3.14	4.22	3.24	3.46	3.89	4.00	5.08	4.87	3.68
TR705	64.58	1.57	1.83	1.31	2.35	1.57	2.09	2.09	3.39	3.91	3.65
TR708	86.48	-0.26	-0.26	-0.13	-0.38	-0.77	-0.26	-0.13	-1.02	-0.77	-0.38
TR710	74.87	1.29	1.03	1.29	0.65	1.16	1.16	1.29	0.90	0.52	0.65
TR712	92.61	0.27	0.40	0.40	0.40	0.13	-0.14	0.40	0.80	0.67	0.27
TR720	57.83	0.25	0.38	0.38	0.76	0.12	0.25	-0.38	0.50	0.25	0.50
TR722	57.09	-0.59	-0.59	-0.40	-0.40	-0.59	0.19	-0.20	-0.20	0.00	-0.40
TR723	85.11	0.77	0.58	0.96	0.00	1.15	0.58	0.77	0.77	1.53	0.58
TR724	59.35	-0.44	-0.22	-0.44	-0.44	-0.44	0.65	-0.87	-1.52	-1.31	-1.31
TR738	90.06	1.71	1.41	1.41	1.71	1.10	1.21	1.21	1.81	2.21	2.11
TR747	82.50	0.56	0.28	0.00	0.00	-0.28	0.28	0.00	-1.11	-1.11	-0.56
TR750	76.79	2.61	2.61	2.06	2.74	2.88	3.02	1.78	2.61	2.61	2.61
TR752	90.37	0.17	0.00	0.00	-0.51	-0.17	-0.17	0.17	-1.18	-0.67	-0.67
TR754	77.94	0.37	-0.37	-0.37	0.00	-0.37	-0.73	-0.73	-8.01	-8.74	-6.56
SUM		21.01	15.19	19.41	16.53	14.82	20.09	19.61	4.240	5.780	7.680
AVG		0.75	0.54	0.69	0.59	0.53	0.72	0.70	0.151	0.206	0.274

Table S14: Initial RMSD (in Å) and Δ RMSD (in Å) results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	2.712	0.008	-0.004	0.021	-0.021	0.009	0.027	0.021	-0.088	-0.120	-0.086
TR655	3.970	-0.007	-0.023	0.015	-0.032	-0.006	0.030	0.005	-0.163	-0.161	-0.159
TR661	2.743	-0.022	-0.008	-0.002	-0.006	0.002	-0.005	-0.007	-0.026	-0.028	0.029
TR662	1.920	-0.022	-0.022	-0.025	-0.033	-0.010	-0.021	-0.023	0.034	0.030	0.050
TR663	3.372	0.013	0.009	0.025	-0.005	0.024	0.023	0.027	-0.034	-0.014	0.011
TR671	7.716	0.092	0.100	0.085	0.123	0.086	0.079	0.095	-0.011	-0.019	-0.021
TR674	3.444	0.055	0.061	0.041	0.040	0.083	0.046	0.035	0.140	0.175	0.153
TR679	3.949	-0.056	-0.057	-0.042	-0.046	-0.067	-0.034	-0.047	0.017	0.018	0.009
TR681	2.305	-0.043	-0.037	-0.036	-0.040	-0.024	-0.029	-0.036	0.379	0.383	0.391
TR688	2.524	-0.005	-0.011	0.006	-0.012	-0.003	0.011	0.006	0.014	0.018	0.000
TR689	1.573	-0.010	-0.005	-0.010	0.010	-0.014	-0.025	0.013	0.033	0.041	0.044
TR696	3.519	0.025	0.040	0.023	0.085	0.036	0.029	0.018	-0.047	-0.042	-0.058
TR698	4.653	-0.020	-0.029	-0.025	-0.039	-0.012	-0.015	-0.030	-0.683	-0.688	-0.678
TR699	2.211	-0.011	0.025	-0.036	0.036	0.018	-0.037	-0.034	0.020	0.027	0.028
TR704	2.540	-0.142	-0.134	-0.147	-0.128	-0.129	-0.139	-0.148	-0.201	-0.153	-0.109
TR705	4.709	0.031	0.060	0.009	0.072	0.043	0.024	0.000	-0.076	-0.075	-0.024
TR708	4.626	0.094	0.100	0.084	0.087	0.114	0.074	0.097	0.136	0.082	-0.005
TR710	2.440	-0.001	-0.001	0.009	0.003	0.005	0.015	0.008	-0.043	-0.032	-0.011
TR712	1.992	0.014	0.025	0.004	0.034	0.018	0.013	0.004	0.034	0.026	0.037
TR720	8.515	0.058	0.066	0.051	0.062	0.063	0.051	0.060	0.231	0.213	0.201
TR722	4.422	0.044	0.043	0.039	0.042	0.044	0.033	0.054	0.071	0.084	0.079
TR723	2.232	-0.022	-0.012	-0.037	0.009	-0.034	-0.046	-0.021	0.057	0.077	0.065
TR724	5.951	0.040	0.051	0.033	0.064	0.039	0.030	0.038	0.031	0.032	0.050
TR738	1.396	-0.109	-0.102	-0.103	-0.090	-0.097	-0.090	-0.104	-0.170	-0.189	-0.203
TR747	1.956	0.006	0.013	0.010	0.009	0.029	0.003	0.025	0.098	0.121	0.100
TR750	2.125	-0.122	-0.126	-0.119	-0.128	-0.117	-0.124	-0.112	-0.131	-0.122	-0.130
TR752	1.495	-0.019	-0.003	-0.033	0.012	-0.016	-0.024	-0.041	-0.016	-0.058	-0.037
TR754	2.410	-0.123	-0.083	-0.144	-0.076	-0.075	-0.135	-0.135	0.152	0.163	0.100
SUM		-0.254	-0.064	-0.304	0.032	0.009	-0.236	-0.232	-0.242	-0.211	-0.174
AVG		-0.009	-0.002	-0.011	0.001	0.000	-0.008	-0.008	-0.009	-0.008	-0.006

Table S15: Initial GDT_HA scores, and Δ GDT_HA results of our CASP12 protocols for CASP10 refinement targets, along with our ProQ2 model selection results. We selected 40%, 20%, and 10% low DFIRE energy (E_{DFIRE}) structures from the last 2 ns trajectory. All results are in GDT_HA unit.

CASP10 Targets	Start GDT_TS	MD0	MD1	MD2	MD1.1	MD1.2	MD2.1	MD2.2	40% of 2ns	20% of 2ns	10% of 2ns
TR644	66.84	2.66	1.95	2.66	1.25	2.66	2.84	2.31	0.54	0.71	-0.35
TR655	60.33	-0.66	-0.83	-0.66	-0.16	-0.83	-0.83	-1.00	-0.16	0.67	1.17
TR661	59.46	2.30	1.62	1.62	1.22	1.89	1.49	1.35	-0.27	1.49	-0.41
TR662	60.33	2.00	1.67	2.67	2.00	1.67	3.34	2.34	1.00	0.67	2.00
TR663	49.34	-0.49	0.17	-0.66	-0.33	-0.16	-0.66	0.00	0.17	-0.33	-0.16
TR671	36.65	0.57	0.28	0.85	0.28	1.13	0.57	1.13	0.85	0.85	1.42
TR674	70.45	3.98	3.79	3.22	4.36	3.41	3.22	3.22	2.87	1.19	1.38
TR679	51.26	1.38	2.01	1.00	2.51	2.13	0.00	1.76	2.01	1.88	1.63
TR681	57.46	2.36	1.96	2.36	1.44	1.96	1.83	2.75	-1.75	-1.62	-1.24
TR688	56.89	2.16	2.30	2.16	2.30	2.43	2.57	2.43	3.38	3.11	3.38
TR689	72.99	-2.02	-2.26	-2.26	-1.90	-2.49	-2.14	-2.49	-4.15	-4.27	-2.37
TR696	50.25	0.50	-2.00	2.50	-2.75	-1.25	1.75	2.25	2.75	2.75	3.25
TR698	44.54	0.63	0.42	1.05	0.84	-0.21	1.05	0.84	1.40	1.61	1.19
TR699	64.44	3.12	3.12	2.23	2.45	3.23	2.78	1.89	-0.77	-0.22	0.45
TR704	48.48	3.90	3.14	4.66	3.47	3.68	4.23	4.44	5.96	5.74	3.90
TR705	43.75	1.82	2.08	1.56	3.39	1.56	2.60	2.60	5.47	5.99	5.99
TR708	72.19	0.39	0.39	0.90	0.26	0.13	0.64	0.77	-1.02	-0.89	0.26
TR710	53.61	1.67	1.03	2.19	0.64	1.29	1.67	2.19	2.70	2.45	2.45
TR712	80.51	1.08	0.54	1.48	0.40	0.27	0.27	0.81	-0.13	0.00	-0.40
TR720	39.77	0.89	1.01	1.01	1.14	0.51	0.63	-0.38	1.14	0.63	0.76
TR722	38.19	-0.59	-0.39	-0.20	-0.20	-0.79	0.20	0.20	-0.20	-0.20	-0.20
TR723	66.03	2.48	2.67	2.67	1.53	3.44	2.48	3.44	1.53	2.48	0.76
TR724	41.52	0.44	0.65	0.00	0.65	0.87	1.52	-0.22	-1.74	-1.52	-1.52
TR738	74.20	3.61	3.21	3.41	3.81	2.21	2.81	3.61	3.41	3.71	3.51
TR747	63.33	1.39	0.84	0.28	0.84	1.11	0.84	0.28	-1.66	-0.55	0.56
TR750	55.08	3.99	3.85	3.57	3.71	4.26	4.26	3.30	5.77	5.50	5.50
TR752	75.84	-0.33	-1.18	-0.16	-1.85	-0.33	-0.16	0.00	-2.87	-2.02	-2.36
TR754	58.82	1.47	0.37	0.37	0.37	0.37	0.37	-0.73	-9.54	-10.27	-8.10
SUM		40.70	32.41	40.48	31.67	34.15	40.17	39.09	16.690	19.540	22.45

Table S16: Energy decomposition comparison for the MD0 model and Minimized-MD model for CASP10 refinement targets.

Target	EAMBER		Bond		Angle		Dihedral		VDWAALS		EEL	
	MD0	Mini-MD	MD0	Min-MD	MD0	Min-MD	MD0	Min-MD	MD0	Min-MD	MD0	Min-MD
TR644	-4433.234	-4629.760	61.380	71.168	273.518	270.538	1789.690	1680.013	-1032.199	-1077.600	-8181.016	-8176.127
TR655	-6806.160	-7144.153	99.671	112.326	376.364	385.985	2140.853	1961.539	-1283.515	-1365.033	-9741.088	-9666.357
TR661	-6745.318	-7289.528	131.839	109.744	464.953	323.023	2356.646	2166.376	-1426.732	-1475.179	-13542.693	-13430.321
TR662	-2907.720	-3088.706	43.197	44.609	179.910	171.713	925.212	832.466	-582.105	-581.709	-4385.191	-4416.563
TR663	-5803.508	-6168.117	75.479	86.658	349.906	301.418	1983.465	1801.051	-1199.266	-1255.395	-11104.049	-11071.574
TR671	-2293.311	-2597.589	40.719	47.997	217.268	158.073	1127.832	1014.488	-495.000	-535.075	-5977.524	-6132.599
TR674	-4013.085	-4252.332	69.001	75.742	330.754	312.600	1575.459	1484.791	-1058.185	-1084.104	-8086.914	-8133.850
TR679	-6403.869	-6834.219	112.010	129.099	529.444	539.888	2782.668	2559.051	-1836.272	-1873.292	-15570.681	-15464.436
TR681	-6161.946	-6834.041	117.258	130.272	523.670	365.767	2771.858	2518.883	-1567.110	-1661.277	-15822.989	-15636.350
TR688	-5612.983	-5843.645	92.510	111.180	426.290	446.316	2350.498	2187.780	-1468.278	-1498.921	-13127.021	-12981.243
TR689	-7243.955	-7908.770	134.337	125.156	627.358	390.222	2917.152	2744.876	-1812.499	-1921.522	-16243.094	-16305.123
TR696	-2815.743	-3008.727	49.249	58.481	276.498	285.883	1253.612	1169.328	-661.590	-719.142	-6721.349	-6684.387
TR698	-3215.293	-3740.790	56.744	63.470	398.362	199.887	1524.399	1378.360	-943.976	-985.160	-9173.653	-9300.281
TR699	-8046.269	-8785.962	143.855	146.527	618.448	456.495	2966.665	2690.917	-1841.979	-1927.363	-16535.506	-16659.296
TR704	-8494.986	-8979.833	150.335	159.127	607.776	567.980	2813.839	2546.109	-1855.884	-1899.995	-14245.288	-14439.251
TR705	-3442.915	-3824.145	70.370	60.811	252.453	192.625	1242.417	1101.484	-600.194	-662.185	-6470.914	-6397.348
TR708	-5915.302	-6300.988	95.668	116.011	548.573	470.308	2360.298	2161.333	-1548.757	-1568.352	-13425.923	-13321.829
TR710	-6179.357	-6425.027	89.579	103.059	302.657	307.039	2324.688	2179.478	-1568.411	-1580.257	-15231.856	-15125.878
TR712	-5423.968	-5610.723	87.454	98.968	389.495	406.197	2267.452	2130.101	-1483.321	-1497.983	-12388.378	-12414.795
TR720	-6558.830	-7151.320	136.196	131.690	567.825	463.553	2560.903	2347.183	-1514.843	-1612.322	-14334.998	-14441.898
TR722	-5445.848	-5721.671	69.775	77.973	243.619	233.881	1690.675	1549.574	-930.074	-942.515	-9017.606	-9174.150
TR723	-4695.297	-4918.716	77.813	82.651	312.113	296.759	1671.407	1563.313	-1108.882	-1145.828	-8986.110	-8938.140
TR724	-3250.040	-3390.286	50.619	61.997	184.893	192.543	1292.628	1230.774	-745.923	-782.351	-7064.020	-7075.972
TR738	-7190.923	-7698.206	119.736	140.061	510.960	447.992	2989.285	2748.995	-1942.668	-2016.268	-17303.205	-17230.203
TR747	-2830.138	-3039.514	47.013	57.034	185.105	191.424	1228.550	1126.681	-684.971	-749.385	-7239.493	-7243.917
TR750	-5153.731	-5418.034	92.823	99.728	394.270	397.087	2145.209	1956.710	-1452.535	-1471.138	-12160.601	-12061.658
TR752	-5153.159	-5376.007	87.375	89.220	395.493	412.664	1816.124	1681.546	-1186.552	-1229.402	-9766.836	-9658.431
TR754	-3082.293	-3255.226	48.125	50.457	200.600	191.273	828.179	776.646	-444.536	-488.585	-4255.072	-4296.505
Target	EGB				1-4 VDW		1-4 EEL		Restraint		NMR Restraints	
TR644	-4878.606	-4782.413	513.412	446.176	7020.586	6938.486	22.607	45.745	4.974	8.680	4.974	8.680
TR655	-4735.015	-4714.503	611.874	511.841	5724.696	5630.050	66.437	92.164	2.453	4.607	2.453	4.607
TR661	-2508.964	-2545.489	715.996	578.974	7063.637	6983.345	22.819	46.017	1.791	4.828	1.791	4.828
TR662	-2573.413	-2560.896	285.973	240.595	3198.697	3181.079	11.414	18.666	0.000	0.000	0.000	0.000
TR663	-4714.492	-4637.668	583.190	489.938	8222.259	8117.455	70.427	91.039	8.056	11.141	8.056	11.141
TR671	-1945.017	-1804.169	312.861	253.048	4425.549	4400.648	27.389	43.873	1.967	3.838	1.967	3.838
TR674	-3187.557	-3133.565	482.126	424.894	5862.231	5801.160	30.591	46.220	4.045	6.499	4.045	6.499
TR679	-3861.419	-3955.343	875.433	735.137	10564.949	10495.677	45.908	82.496	1.680	3.643	1.680	3.643
TR681	-3246.728	-3331.286	830.483	687.165	10231.611	10092.787	53.300	80.516	9.369	17.009	9.369	17.009
TR688	-2686.260	-2758.714	642.566	574.096	8156.712	8075.862	28.865	46.046	1.091	2.802	1.091	2.802
TR689	-4652.738	-4533.299	883.679	750.069	10901.850	10840.851	40.277	65.907	11.673	22.236	11.673	22.236
TR696	-1754.199	-1765.630	363.128	298.257	4378.909	4348.483	33.182	50.795	2.909	6.337	2.909	6.337
TR698	-2074.727	-1983.273	472.341	384.777	6525.217	6501.431	16.679	31.107	0.000	0.000	0.000	0.000
TR699	-4662.465	-4490.857	951.600	781.594	10313.114	10216.021	43.872	72.018	4.573	7.686	4.573	7.686
TR704	-3134.496	-2925.371	846.039	727.190	6322.693	6284.379	68.599	91.359	6.778	11.632	6.778	11.632
TR705	-2332.392	-2370.747	361.854	280.387	4033.490	3970.829	30.723	50.585	2.019	2.962	2.019	2.962
TR708	-2422.859	-2437.304	677.456	587.671	7800.242	7691.175	36.580	50.171	4.361	5.686	4.361	5.686
TR710	-3130.652	-3192.580	688.203	601.481	10346.435	10282.632	11.650	28.243	0.000	0.000	0.000	0.000
TR712	-3995.514	-3870.820	642.885	578.547	9055.958	8959.062	25.248	48.133	6.480	14.163	6.480	14.163
TR720	-3126.299	-2974.419	814.864	668.015	8337.522	8266.878	30.800	56.676	3.938	6.082	3.938	6.082
TR722	-2929.558	-2798.585	499.954	409.617	4927.368	4922.536	7.793	20.788	0.000	0.000	0.000	0.000
TR723	-2199.243	-2215.592	505.294	446.910	5032.310	4991.211	20.790	32.107	0.000	0.000	0.000	0.000
TR724	-1803.916	-1791.883	386.231	333.479	4449.449	4441.127	38.514	57.752	5.024	7.131	5.024	7.131
TR738	-3225.025	-3242.622	885.644	761.764	10774.351	10692.074	37.412	61.918	1.884	3.041	1.884	3.041
TR747	-1633.567	-1564.056	384.182	316.281	4883.042	4826.423	22.551	32.377	5.477	6.567	5.477	6.567
TR750	-2376.178	-2383.721	594.231	522.532	7609.051	7522.426	31.462	49.769	1.430	2.964	1.430	2.964
TR752	-2898.710	-2971.455	522.507	461.799	5877.441	5838.051	23.271	44.758	6.985	10.900	6.985	10.900
TR754	-1421.939	-1367.688	261.670	203.898	1700.680	1675.278	17.935	34.277	0.000	0.000	0.000	0.000

Table S17: Radius of gyration of the MD0 model and Minimized-MD model for CASP10 refinement targets.

Target	Length	MD0	Minimized-MD
TR644	141	16.638	16.614
TR655	175	15.592	15.560
TR661	185	17.220	17.197
TR662	75	11.369	11.353
TR663	152	16.220	16.201
TR671	88	15.801	15.889
TR674	132	14.049	14.069
TR679	223	17.273	17.299
TR681	224	22.991	23.060
TR688	185	17.575	17.589
TR689	234	19.627	19.566
TR696	100	14.210	14.245
TR698	119	13.541	13.558
TR699	234	18.483	18.448
TR704	235	18.795	18.778
TR705	96	13.762	13.779
TR708	196	16.044	16.020
TR710	194	19.575	19.640
TR712	186	16.585	16.589
TR720	202	18.576	18.532
TR722	127	34.337	34.340
TR723	132	14.422	14.406
TR724	113	14.470	14.469
TR738	249	17.870	17.902
TR747	98	13.489	13.470
TR750	182	15.282	15.284
TR752	156	15.780	15.746
TR754	68	12.218	12.128
AVG		16.638	16.614

Table S18: Model quality comparison of the starting targets, MD0 and Minimized-MD models for CASP10 refinement targets. All results are obtained by using the WHAT-CHECK program.

Target	Start	MD0	Minimized-MD
TR644	-0.054	-0.522	-1.163
TR655	-2.373	-1.526	-2.137
TR661	0.232	0.225	-0.458
TR662	0.412	-0.155	-0.650
TR663	0.098	-0.117	-1.159
TR671	-2.986	-2.566	-3.114
TR674	-0.453	-1.552	-1.967
TR679	-0.469	-1.023	-1.613
TR681	-1.972	-2.086	-2.489
TR688	-0.041	-0.657	-1.047
TR689	-0.096	-0.581	-1.149
TR696	-2.308	-2.708	-3.099
TR698	0.674	-0.216	-0.776
TR699	-0.228	-0.758	-1.618
TR704	-2.119	-2.156	-2.481
TR705	-2.054	-2.220	-2.529
TR708	-0.451	-1.807	-2.158
TR710	0.170	-0.087	-0.480
TR712	-0.854	-1.261	-1.693
TR720	-1.152	-1.377	-1.730
TR722	3.363	3.204	2.103
TR723	1.087	-0.094	-0.533
TR724	-2.921	-4.007	-4.088
TR738	0.356	-0.662	-1.261
TR747	0.439	-0.638	-1.154
TR750	-0.371	-0.088	-0.950
TR752	0.378	-0.409	-0.858
TR754	-3.347	-3.359	-4.244
AVG	-0.609	-1.043	-1.589

Table S19: Δ GDT_TS comparison between MD0 model and Minimized-MD model.

Target	MD0	Minimized-MD
TR644	0.890	-1.060
TR655	-1.670	-2.830
TR661	1.350	-0.680
TR662	1.340	1.340
TR663	-0.490	-0.170
TR671	0.570	-1.700
TR674	1.700	0.750
TR679	1.130	0.120
TR681	0.790	-0.910
TR688	1.480	0.270
TR689	-0.240	-1.310
TR696	0.250	0.500
TR698	0.630	0.210
TR699	1.220	-1.330
TR704	3.780	2.490
TR705	1.570	1.830
TR708	-0.260	-0.890
TR710	1.290	0.900
TR712	0.270	-1.350
TR720	0.250	-1.140
TR722	-0.590	1.370
TR723	0.770	0.200
TR724	-0.440	-0.440
TR738	1.710	1.000
TR747	0.560	-2.780
TR750	2.610	0.680
TR752	0.170	-0.670
TR754	0.370	-3.680
AVG	0.750	-0.331

Table S20: Group information for top ranked model in CASP11. LEE and RFMQA models (TR283, TR811, TR817) are from our group.

targets	Model from
TR217	MUFOLD-R
TR274	Boniecki_pred
TR280	Schroderlab
TR283	RFMQA
TR759	Anthropic_Dreams
TR760	Seok-refine
TR762	Boniecki_pred
TR765	FEIG
TR768	Jones-UCL
TR769	Schroderlab
TR772	FEIG
TR774	FEIG
TR776	FEIG
TR780	Schroderlab
TR782	FEIG
TR783	FEIG
TR786	Schroderlab
TR792	FEIG
TR803	BAKER
TR810	Seok-refine
TR811	LEE
TR816	SHORTLE
TR817	RFMQA

Table S21: Side chain accuracy (in terms of χ_1 and χ_2 , in percentage, using 30 degree criteria) for CASP10 starting targets, MD0 and minimized-MD model.

Target	χ_1 accuracy			χ_2 accuracy		
	Start	MD0	Minimized-MD	Start	MD0	Minimized-MD
TR644	60.00	60.83	59.17	50.57	47.13	42.53
TR655	51.28	50.43	51.28	44.12	41.18	41.18
TR661	56.21	52.29	58.17	30.58	26.45	28.93
TR662	51.47	41.18	45.59	22.92	20.83	18.75
TR663	60.76	64.96	64.96	42.42	41.23	31.58
TR671	36.99	49.32	46.58	24.53	33.96	28.30
TR674	53.70	54.63	57.41	42.68	46.34	51.22
TR679	55.62	45.56	52.66	41.91	28.68	38.97
TR681	59.76	56.52	53.42	44.83	41.59	42.48
TR688	64.02	60.98	61.59	52.80	44.00	46.40
TR689	55.80	60.77	55.80	40.16	52.76	40.94
TR696	41.38	41.38	41.38	37.10	33.87	30.65
TR698	61.39	49.51	54.37	38.57	31.43	35.71
TR699	45.54	49.50	48.51	28.30	30.19	27.04
TR704	64.00	63.43	65.14	46.32	50.00	49.26
TR705	62.20	40.24	46.34	30.16	20.63	23.81
TR708	71.88	66.87	68.12	55.37	47.93	51.24
TR710	69.33	64.67	63.33	53.28	50.82	51.64
TR712	66.23	68.18	71.43	52.99	56.41	55.56
TR720	62.50	52.84	48.30	51.47	34.56	33.09
TR722	49.07	38.89	44.44	36.59	21.95	23.17
TR723	55.65	60.87	62.61	43.68	42.53	41.38
TR724	47.78	38.89	41.11	25.86	32.76	31.03
TR738	69.90	65.31	68.37	51.43	45.71	47.14
TR747	59.76	50.00	52.44	44.07	33.90	37.29
TR750	64.06	57.81	57.81	55.21	42.71	39.58
TR752	63.56	56.78	63.56	51.72	43.68	52.87
TR754	42.19	35.94	46.87	22.45	16.33	18.37
AVG	57.22	53.52	55.38	41.50	37.84	37.86

Table S22: Δ GDT_TS decomposition for CASP10 targets for MD0 model.

Target	GDT_TS	%(d<1)	%(d<2)	%(d<4)	%(d<8)
TR644	0.89	2.12	1.42	0.00	0.00
TR655	-1.67	-5.33	-2.00	0.00	0.67
TR661	1.35	4.86	0.54	0.00	0.00
TR662	1.34	4.00	1.33	0.00	0.00
TR663	-0.49	-1.32	-1.32	0.00	0.66
TR671	0.57	0.00	0.00	2.28	0.00
TR674	1.70	6.06	0.00	0.76	0.00
TR679	1.13	2.52	1.51	0.50	0.00
TR681	0.79	5.24	-2.10	0.00	0.00
TR688	1.48	5.95	0.54	-0.54	0.00
TR689	-0.24	-2.85	1.42	0.48	0.00
TR696	0.25	-1.00	1.00	1.00	0.00
TR698	0.63	1.68	0.84	0.00	0.00
TR699	1.22	5.34	-0.45	0.00	0.00
TR704	3.78	5.20	7.35	2.60	0.00
TR705	1.57	5.21	0.00	2.09	-1.04
TR708	-0.26	-0.51	-0.51	0.00	0.00
TR710	1.29	3.61	1.04	0.52	0.00
TR712	0.27	1.61	0.54	-0.53	-0.54
TR720	0.25	1.52	0.51	-0.50	-0.51
TR722	-0.59	-0.79	0.00	-0.79	-0.78
TR723	0.77	2.29	1.52	0.00	-0.76
TR724	-0.44	0.87	-1.74	-0.87	0.00
TR738	1.71	4.42	2.41	0.00	0.00
TR747	0.56	2.22	-1.11	1.11	0.00
TR750	2.61	6.05	2.75	1.65	0.00
TR752	0.17	0.00	0.68	0.00	0.00
TR754	0.37	0.00	0.00	1.47	0.00
AVG	0.75	2.11	0.58	0.40	-0.08