Structure, Volume *19*

Supplemental Information

Atomic-Level Protein Structure Refinement Using Fragment-Guided Molecular Dynamics Conformation Sampling

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Inventory of Supplemental Information

Table S1: This table provides a full list of CASP8 refinement groups and is cited in the third section of RESULTS AND DISCUSSIONS.

Table S2: This table provides a full list of CASP9 refinement groups and is cited in the fourth section of RESULTS AND DISCUSSIONS.

Figure S1: This figure provides a histogram of the score differences of templates and is cited in first section of RESULTS AND DISCUSSIONS.

Figure S2: This figure shows an example of contrast energy landscape and is cited in first section of RESULTS AND DISCUSSIONS.

Figure S3: This figure shows the restraint accuracy in different categories and is cited in second section of RESULTS AND DISCUSSIONS.

Supporting Information

Supplementary Tables

Table S1, related to Table 2. Refinement results on 12 proteins from the CASP8 experiment.

Group	#targ[a]	GDT[b]	TM[c]	HB[d]	#Clash[e]	Molprob[f]
FG-MD	12	6.979	9.362	6.758	0.08	2.575
NULL[g]	12	6.898	9.316	6.29	27.92	2.706
LEE	12	6.860	9.195	6.624	18.42	2.613
LevittGroup	12	6.701	9.160	6.730	5.25	2.875
FAMSD	12	6.562	8.746	6.149	0.50	2.796
SAM-T08-human	12	6.523	9.084	6.773	0.67	2.762
YASARARefine	12	6.407	9.155	6.853	0.25	1.071
Bates_BMM	12	6.167	8.734	6.060	2.92	2.737
FEIG_REFINE	11	6.158	8.462	5.879	2.55	2.192
FAMS-multi	12	6.055	8.281	5.769	2.67	3.420
Abagyan	10	6.054	8.262	5.353	10.70	3.136
xianmingpan	11	5.977	8.474	5.929	0.18	1.698
A-TASSER	11	5.751	8.133	5.764	9.09	2.597
POISE	12	5.556	8.376	5.675	0.58	1.844
SAMUDRALA	10	5.441	7.190	4.816	5.70	2.329
DBAKER	9	5.413	7.041	5.371	9.44	1.636
MidwayFolding	10	5.273	7.251	5.128	57.40	3.528
Jones-UCL	12	5.175	8.089	5.617	0.83	3.402
tripos_08	8	4.619	6.295	4.270	0.88	2.826
Elofsson	12	4.596	6.763	4.538	23.33	2.713
jacobson	7	4.288	5.566	3.905	1.29	2.855
Keasar	7	3.552	5.413	4.302	3.71	2.765
POEM	8	2.652	4.356	1.411	11.88	4.304
PS2-server	3	1.646	2.206	1.393	0.33	3.035
EB_AMU_Physics	3	1.610	2.421	1.894	1.00	2.867
TASSER	2	1.131	1.652	1.290	19.00	2.913
Kolinski	1	0.565	0.845	0.546	0.00	2.602

[a] Number of refinement targets

[b] Cumulative TM-score of all submitted first models

[c] Cumulative GDT-HA score of all submitted first models

[d] Cumulative hydrogen bonding score of all submitted first models

[e] Average number of heavy atom steric clash of the first models

[f] Average MolProbity score of first models

[g] Starting models for refinement experiment

Table S2, related to Table 2. Result of 14 target proteins of CASP9 refinement experiment

Group	#targ[a]	GDT[b]	TM[c]	HB[d]	#Clash[e]	MolProb[f]
FG-MD	14	7.387	10.386	6.928	0.00	2.183
ZHANG	14	7.365	10.396	7.084	0.00	3.042
SEOK	14	7.359	10.399	6.819	15.79	3.436
NULL[g]	14	7.319	10.368	6.867	3.71	2.521
FAMSD	14	7.284	10.348	6.79	1.07	2.55
FAMS-MULTI	14	7.284	10.348	6.79	1.07	2.55
KNOWMIN	14	7.194	10.182	7.59	1.21	2.179
TASSER	14	7.164	10.259	6.814	47.43	3.16
BAKER	14	7.156	10.287	7.386	0.14	1.327
SAMUDRALA	14	7.031	10.038	6.875	0.07	2.395
YASARA	14	7.023	10.043	7.314	0.07	0.969
GWS	14	6.962	9.74	6.729	11.07	2.585
LEE	14	6.962	9.74	6.729	11.07	2.751
PCOMB	14	6.876	9.866	7.206	0.07	1.407
GENESILICO	14	6.849	9.994	5.434	25.29	3.633
SHORTLE	14	6.834	10.04	6.024	18.57	3.513
RECOMBINEIT	14	6.779	9.854	5.559	53.21	3.177
PCONS	14	6.631	9.678	7.111	0.21	1.495
FEIG	13	6.612	9.26	6.043	0.00	2.238
PROQ2	14	6.496	9.61	7.032	0.14	1.623
PCONSM	14	6.491	9.57	7.374	0.07	1.343
PROQ	14	6.246	9.454	6.771	0.36	1.542
MIDWAYFOLDINGHUMAN	12	6.203	8.677	5.588	70.08	2.715
SCHRODERLAB	12	6.184	8.768	5.928	0.00	1.718
PHAISTOS	14	6.11	9.509	4.606	0.07	1.845
KEASAR	13	5.935	9.104	6.039	14.08	3.56
BILAB-SOLO	13	5.713	8.471	5.333	52.62	2.864
3SP-TSAILAB	11	5.258	7.951	3.214	102.91	4.012
FOLDIT	10	4.643	6.853	5.001	0.00	1.414
PCONSD	7	3.788	5.345	3.502	5.86	3.581
JONES-UCL	6	3.031	4.287	2.816	0.50	3.315
MIDWAYFOLDINGSERVER	5	2.488	3.65	2.276	63.80	2.333
STRUPPI	9	2.368	3.754	2.182	2.44	3.592
SBTJ	4	2.339	3.128	2.044	5.25	2.949
ZHOU-SPARKS-X	3	1.344	1.982	1.235	268.33	3.581
SWA_TEST	1	0.646	0.887	0.524	1.00	1.798
TMD3D	1	0.351	0.519	0.489	0.00	2.628

[a] Number of refinement targets
[b] Cumulative TM-score of all submitted first models
[c] Cumulative GDT-HA score of all submitted first models
[d] Cumulative hydrogen bonding score of all submitted first models
[e] Average number of heavy atom steric clash of the first models
[f] Average MolProbity score of first models
[g] Starting models for refinement experiment

Supplementary Figures

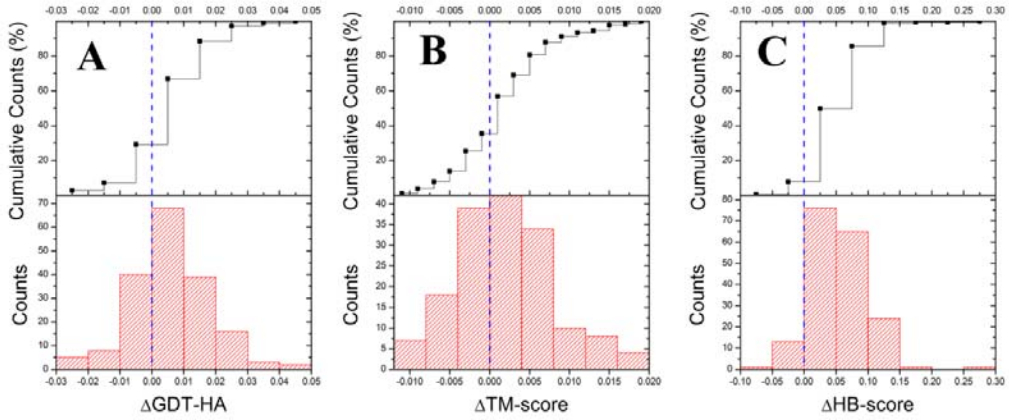

Figure S1, related to Figure 2. The histogram of score difference for 181 benchmark set proteins.

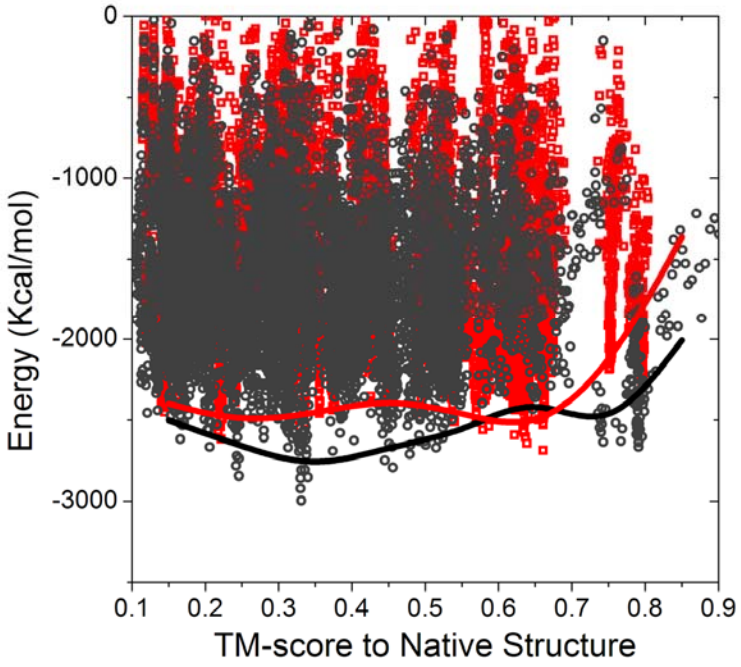

Figure S2, related to Figure 2. An example of failed cases in re-shaping the energy landscape by FG-MD. AMBER99 (black circles) and FG-MD (red squares) energies vs. TM-score for 60×200 refined models (PDB ID 1z3e) by MD and FM-MD simulations.

The fitting curves are connection of the medians of the 10 lowest-energy models in each of the TM-score bins (0.1-0.2, 0.2-0.3, ...).

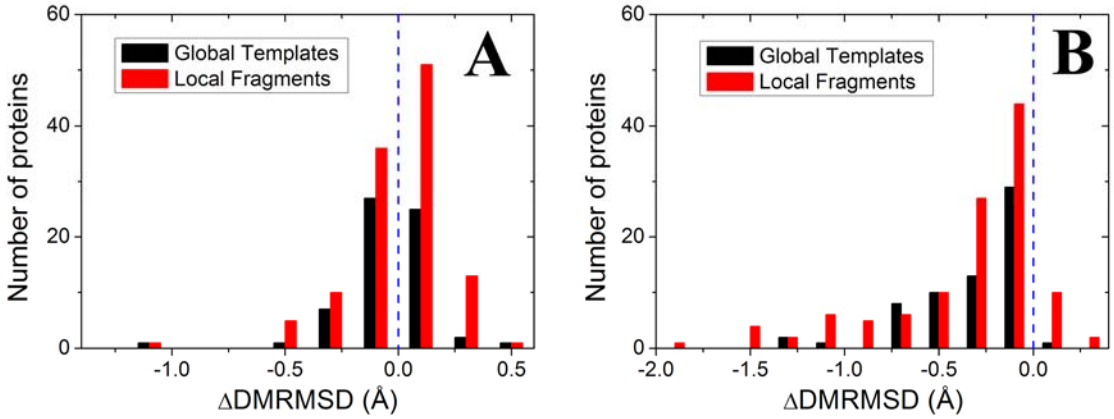

Figure S3, related to Figure 3. Restraint accuracy from global and fragment templates. (A) Histogram of ΔDMRMSD of distance map restraints taken from the global templates (black) and fragmental templates (red) for "successful" refinement cases. (B) Histogram of ΔDMRMSD of distance map restraints taken from the global templates (black) and fragmental templates (red) for "failed" refinement cases.