

## **Supplementary Information**

### **3Drefine: Consistent Protein Structure Refinement by Optimizing Hydrogen-Bonding Network and Atomic-Level Energy Minimization**

**Debswapna Bhattacharya and Jianlin Cheng**

#### **Glossary of Supplementary Information**

**Table S1: This table provides results of 3Drefine and all groups participating in CASP8 Refinement Experiment and is cited in the second section of RESULTS AND DISCUSSIONS.**

**Table S2: This table provides results of 3Drefine and all groups participating in CASP9 Refinement Experiment and is cited in the third section of RESULTS AND DISCUSSIONS.**

**Figure S1: This figure provides a histogram of the score for 107 CASP9 targets and is cited in fifth section of RESULTS AND DISCUSSIONS.**

## Supplementary Tables

**Table S1, related to Table II.** Refinement results for 3Drefine and all the participating groups in CASP8 Refinement Experiment\*.

Group Name	No. of Targets <sup>a</sup>	GDT-HA <sup>b</sup>	TM-score <sup>c</sup>	MolProbity <sup>d</sup>
3Drefine	12	6.932	9.3289	2.349
NULL <sup>e</sup>	12	6.898	9.316	2.706
LEE	12	6.86	9.195	2.613
LevittGroup	12	6.701	9.16	2.875
FAMSD	12	6.562	8.746	2.796
SAM-T08-human	12	6.523	9.084	2.762
YASARARefine	12	6.407	9.155	1.071
Bates_BMM	12	6.167	8.734	2.737
FEIG_REFINE	11	6.158	8.462	2.192
FAMS-multi	12	6.055	8.281	3.42
Abagyan	10	6.054	8.262	3.136
xianmingpan	11	5.977	8.474	1.698
A-TASSER	11	5.751	8.133	2.597
POISE	12	5.556	8.376	1.844
SAMUDRALA	10	5.441	7.19	2.329
DBAKER	9	5.413	7.041	1.636
MidwayFolding	10	5.273	7.251	3.528
Jones-UCL	12	5.175	8.089	3.402
tripos_08	8	4.619	6.295	2.826
Elofsson	12	4.596	6.763	2.713
jacobson	7	4.288	5.566	2.855
Keasar	7	3.552	5.413	2.765
POEM	8	2.652	4.356	4.304
PS2-server	3	1.646	2.206	3.035
EB_AMU_Physics	3	1.61	2.421	2.867
TASSER	2	1.131	1.652	2.913
Kolinski	1	0.565	0.845	2.602

<sup>a</sup> Number of CASP8 targets in the Refinement Experiment.

<sup>b</sup> Cumulative GDT-HA score based on the first submitted model.

<sup>c</sup> Cumulative TM-score based on the first submitted model.

<sup>d</sup> Average MolProbity score based on the first submitted model.

<sup>e</sup> The initial models for the CASP8 refinement experiment.

\* Refinement results for groups other than 3Drefine have been adopted from [1], [2].

**Table S2, related to Table 11.** Refinement results for 3Drefine and all the participating groups in CASP9 Refinement Experiment\*.

<b>Group Name</b>	<b>No. of Targets<sup>a</sup></b>	<b>GDT-HA<sup>b</sup></b>	<b>TM-score<sup>c</sup></b>	<b>MolProbit<sup>d</sup></b>
3Drefine	14	7.388	10.388	2.101
ZHANG	14	7.365	10.396	3.042
SEOK	14	7.359	10.399	3.436
NULL <sup>e</sup>	14	7.319	10.368	2.521
FAMSD	14	7.284	10.348	2.55
FAMS-MULTI	14	7.284	10.348	2.55
KNOWMIN	14	7.194	10.182	2.179
TASSER	14	7.164	10.259	3.16
BAKER	14	7.156	10.287	1.327
SAMUDRALA	14	7.031	10.038	2.395
YASARA	14	7.023	10.043	0.969
GWS	14	6.962	9.74	2.585
LEE	14	6.962	9.74	2.751
PCOMB	14	6.876	9.866	1.407
GENESILICO	14	6.849	9.994	3.633
SHORTLE	14	6.834	10.04	3.513
RECOMBINEIT	14	6.779	9.854	3.177
PCONS	14	6.631	9.678	1.495
FEIG	13	6.612	9.26	2.238
PROQ2	14	6.496	9.61	1.623
PCONSM	14	6.491	9.57	1.343
PROQ	14	6.246	9.454	1.542

<sup>a</sup> Number of CASP9 targets in the Refinement Experiment.

<sup>b</sup> Cumulative GDT-HA score based on the first submitted model.

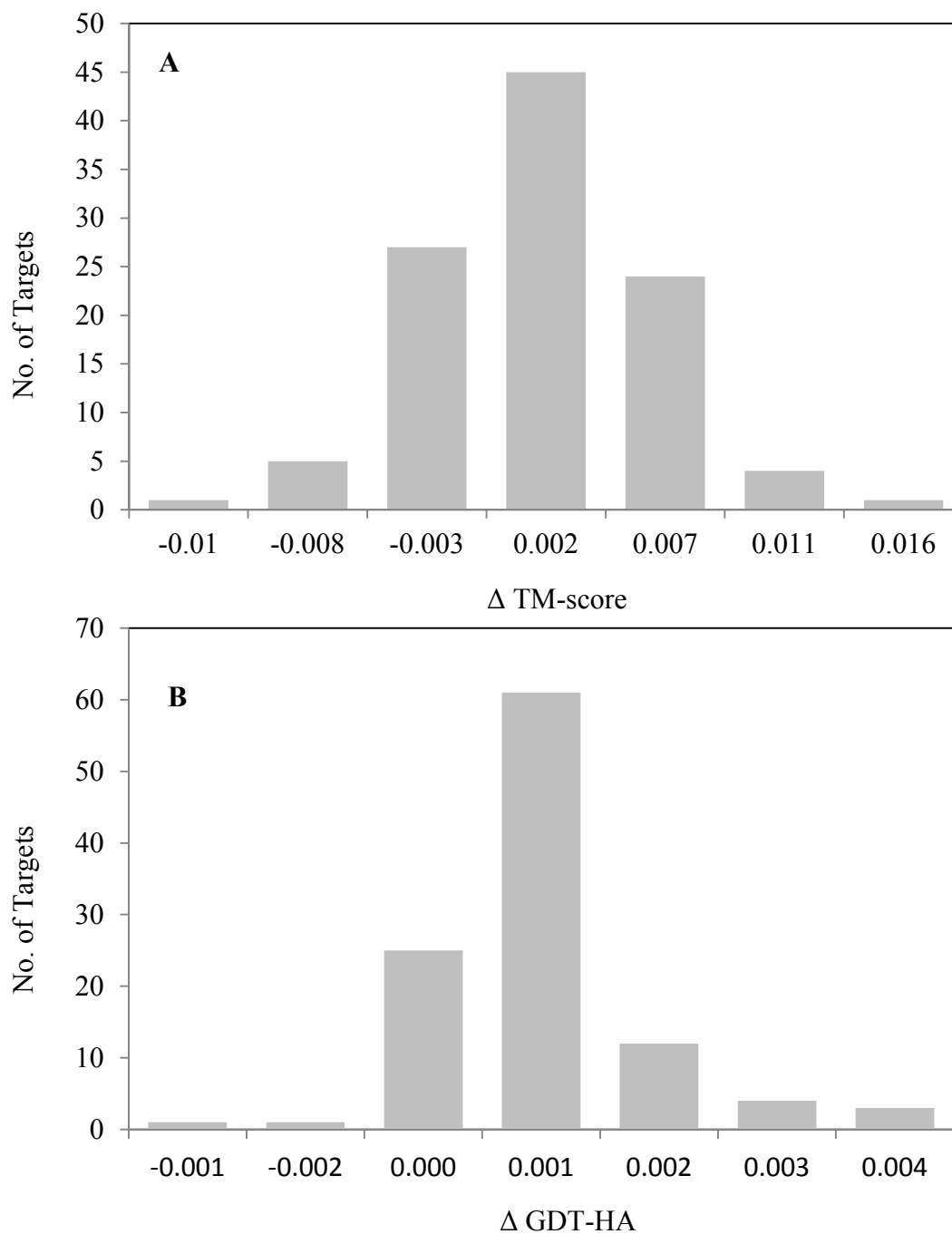
<sup>c</sup> Cumulative TM-score based on the first submitted model.

<sup>d</sup> Average MolProbit score based on the first submitted model.

<sup>e</sup> The initial models for the CASP9 refinement experiment.

\* Refinement results for groups other than 3Drefine have been adopted from [1], [3].

## Supplementary Figures



**Figure S1, related to Figure 5.** The histogram of score changes for 107 CASP9 targets (Initial structures generated using MULTICOM-REFINE).

(A) Histogram for TM-score changes.

(B) Histogram for GDT-HA score changes.

A positive change indicates that the quality of the model of a target was improved by refinement.

## References:

1. Zhang J, Liang Y, Zhang Y (2011). Atomic-Level Protein Structure Refinement Using Fragment-Guided Molecular Dynamics Conformation Sampling. *Structure*, vol 19, 1784-1795.
2. MacCallum JL., Hua L, Schnieders MJ, Pande VS, Jacobson MP, Dill KA (2009). Assessment of the protein-structure refinement category in CASP8. *Proteins* 77 (Suppl 9), 66–80.
3. MacCallum JL, Pe´rez A, Schnieders MJ, Hua L, Matthew, Jacobson P, Dill KA. (2011). Assessment of protein structure refinement in CASP9. *Proteins* 79 (Suppl 10), 74-90.