Supplementary materials

Error estimation guided rebuilding of *de novo* models increases the success rate for *ab initio* phasing

Rojan Shrestha[ab], David Simoncini[a] and Kam Y. J. Zhang[ab]*

[a]Zhang Initiative Research Unit, Advance Science Institute, RIKEN, 2-1 Hirosawa, Wako, Saitama, 351-0198, Japan, and [b]Department of Computational Biology, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-0882, Japan

input : $AP\text{-}RDS$ {vector of scores; $length(AP\text{-}RDS) > 0$}
output : i {index in $AP\text{-}RDS$}
$n \leftarrow length(AP\text{-}RDS)$
$TS \leftarrow sum(AP\text{-}RDS)$
$i \leftarrow 0$
$acc \leftarrow AP\text{-}RDS[i]$
$fortune \leftarrow TS * random(0,1)$
while $(acc < fortune) \wedge (i < n-1)$ **do**
  $i \leftarrow i+1$
  $acc \leftarrow acc + AP\text{-}RDS[i]$
end while
return i

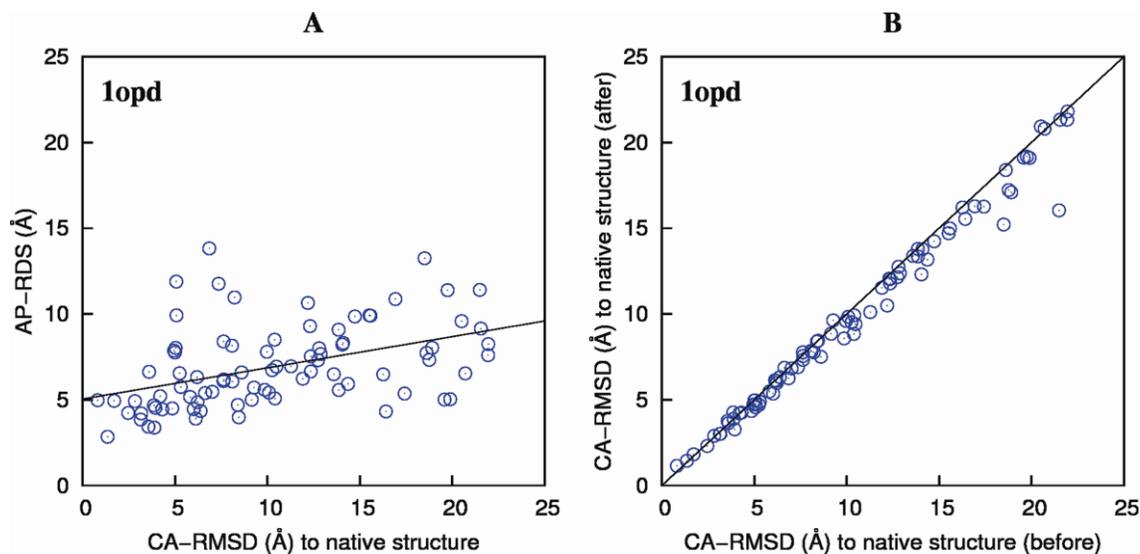Figure S1: The algorithm used to achieve the Roulette wheel procedure.

Figure S2: The correlation between AP-RDS and prediction accuracy for each residue and the model improvement after rebuilding for 1OPD. (A) The correlation between AP-RDS score and the CA-RMSD of each residue in selected models. (B) Improvement in CA-RMSD for each residue in coarse-grained models before and after rebuilding using MORPHEUS.
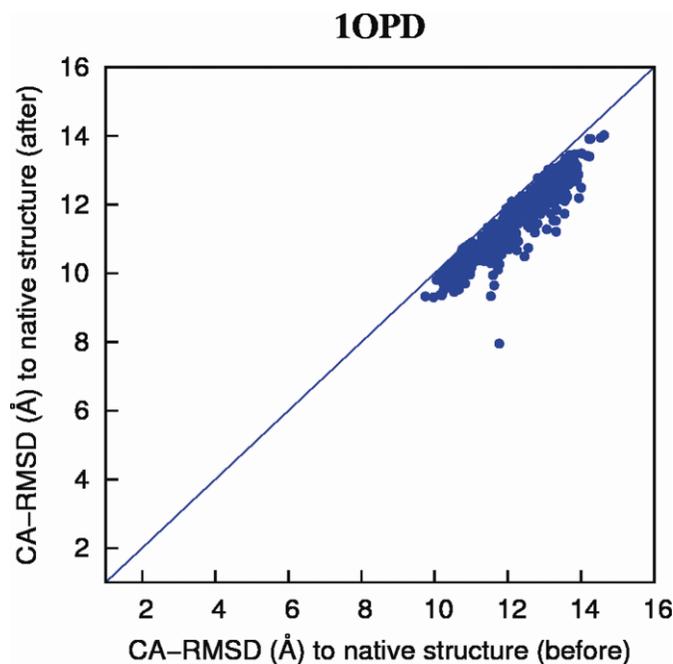

Figure S3: Improvement to the coarse-grained models after rebuilding for 1OPD. A scatter plot of the CA-RMSDs before and after rebuilding for all coarse-grained models is shown. A diagonal line is drawn on each panel. Points below this line represent models with improved CA-RMSD.