



STRUCTURAL
BIOLOGY

Volume 79 (2023)

Supporting information for article:

**Direct phasing algorithm for protein crystals with high solvent
content using low-resolution diffraction data**

**Yu-Meng Jiang, Han Miao, Xin-Yu Pan, Qi Wang, Zheng Dong, Zhi Geng
and Yu-Hui Dong**

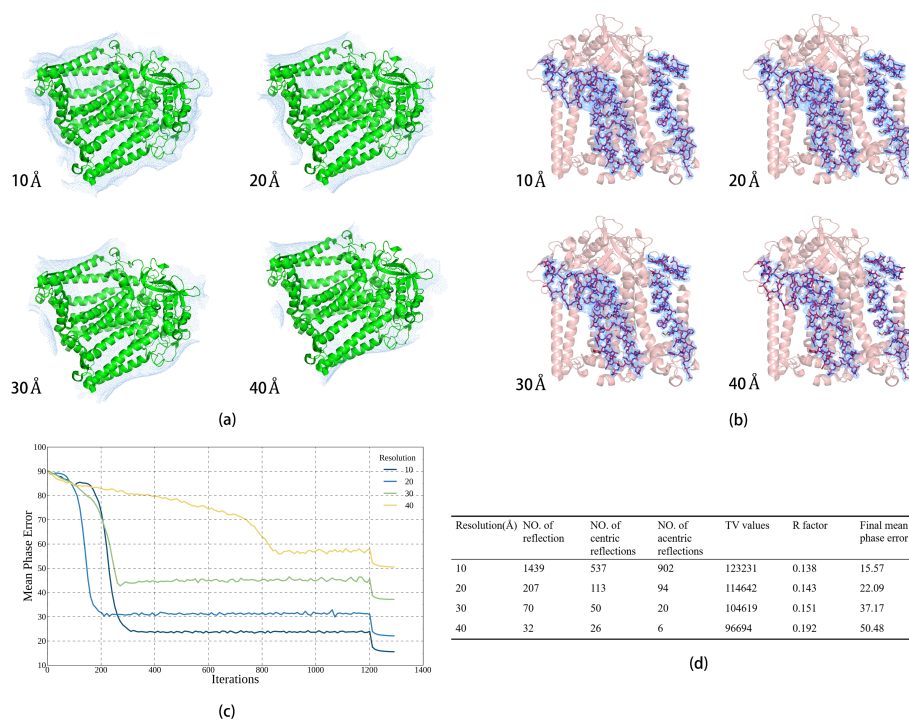


Figure S1 Simulated 2UXJ envelopes at different resolutions and phase retrieval results.

These runs were initiated with random phase sets. (a) 2UXJ envelope at different resolutions (in blue) compared with the atomic model of 2UXJ (in green). (b) recovered density maps (2.0σ) after the 1200 HIO algorithm and 100 ER algorithm (in blue) compared with the atomic model of 2UXJ (in pink) (c) Average errors in phase angles versus the number of iterations of one of the successful runs of 2UXJ. (d) details of 2UXJ envelopes in different resolutions.

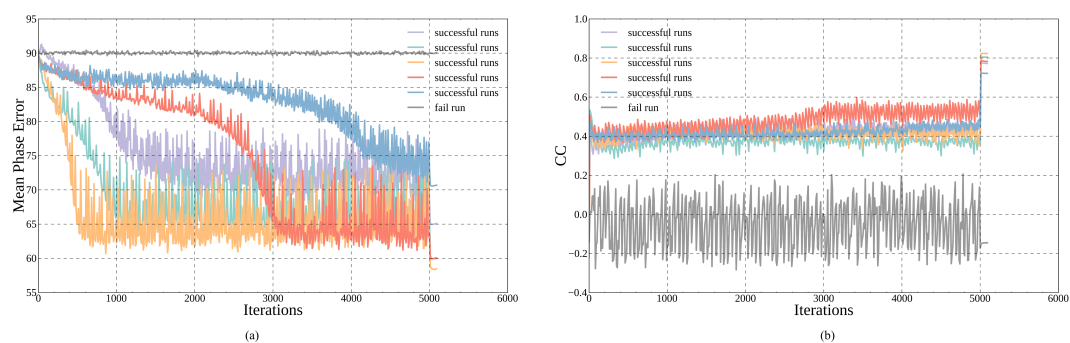


Figure S2 The trajectories of the mean phase error and CC of 2UXJ starting from random phase sets. There were five successful runs. A sudden drop of phase error indicates a convergent run.

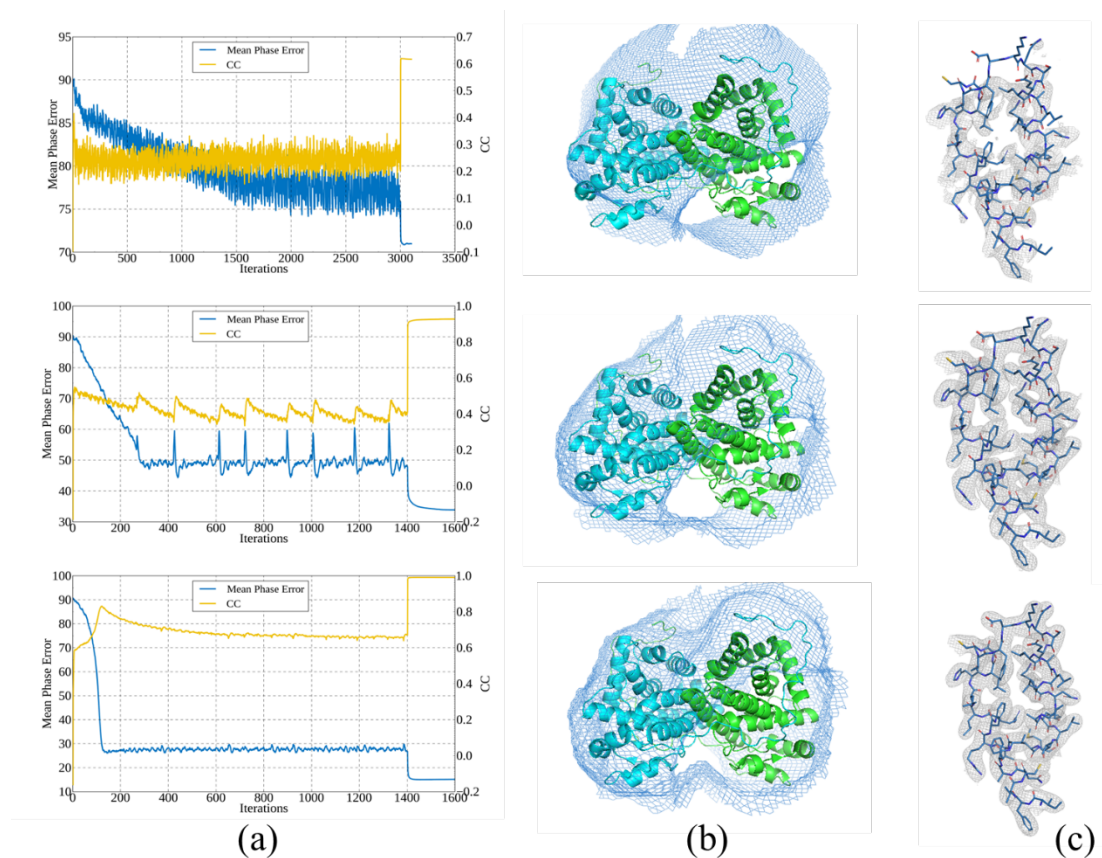


Figure S3 Results of the phasing-dm procedure for 5ZB3.

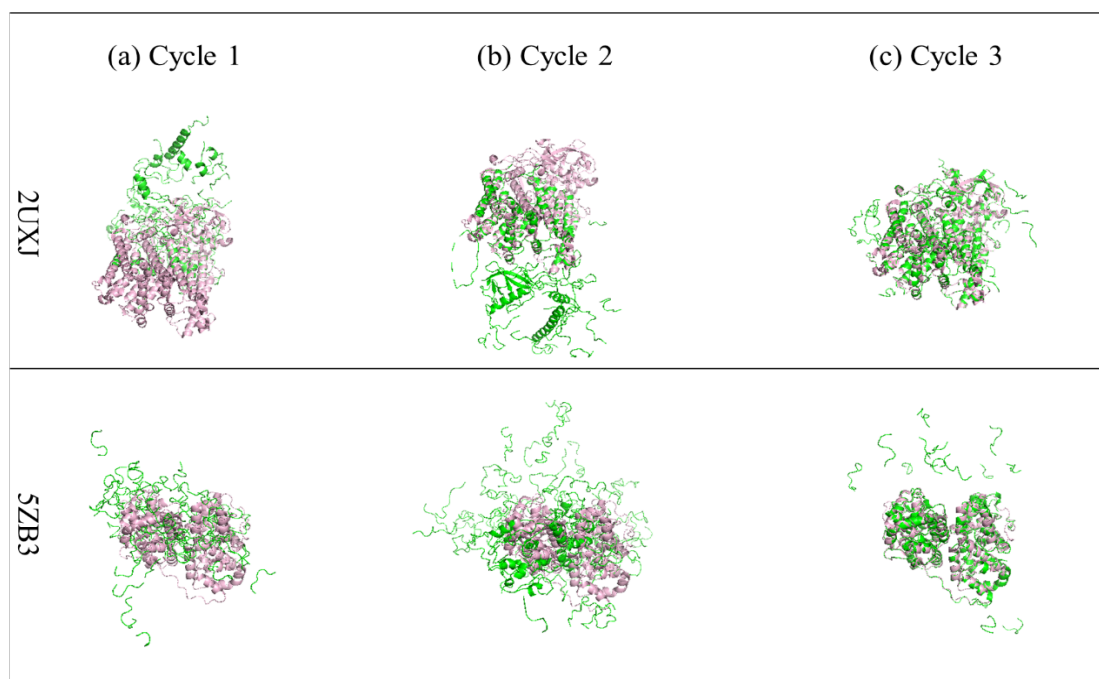


Figure S4 Structure comparison. Models from the workflow (in green) alongside the crystal structures deposited in the PDB (in pink). (a)(b)(c) are calculated models in different cycle versus 2UXJ and 5ZB3 respectively.

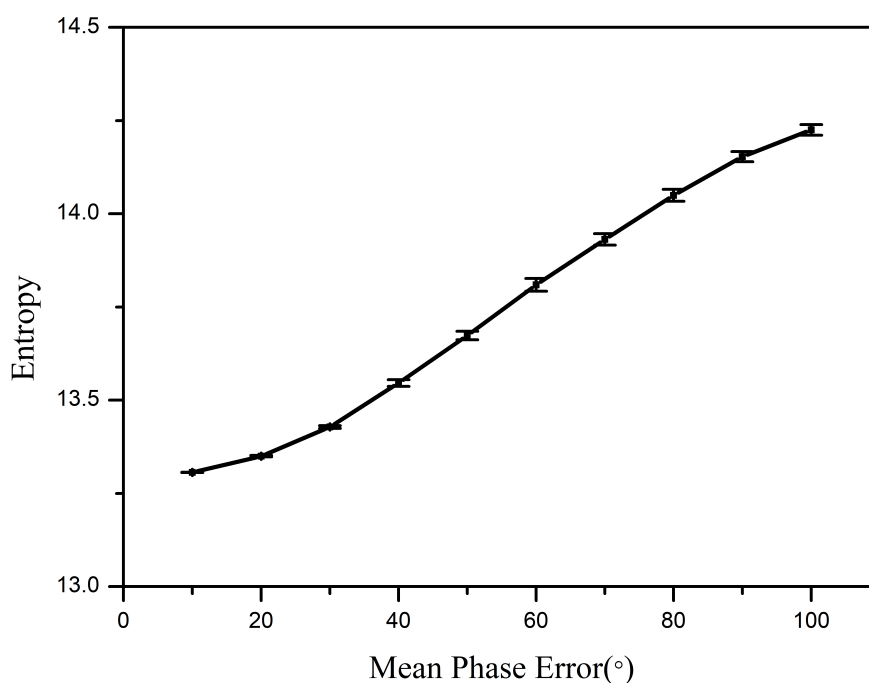


Figure S5 Effect of mean phase error on the entropy of electron density maps, where the phase error is simulated by varying degrees of random error.

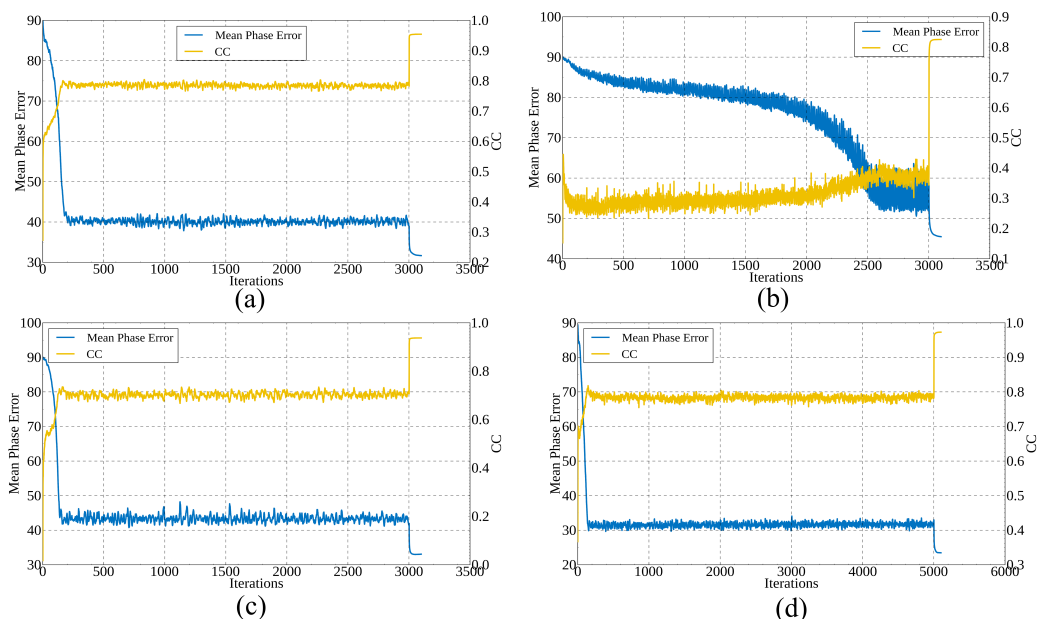


Figure S6 The trajectories of the mean phase error and CC starting from random phase sets.

(a) 1KOA (b) 1BOT (c) 4AVT (d) 7STQ

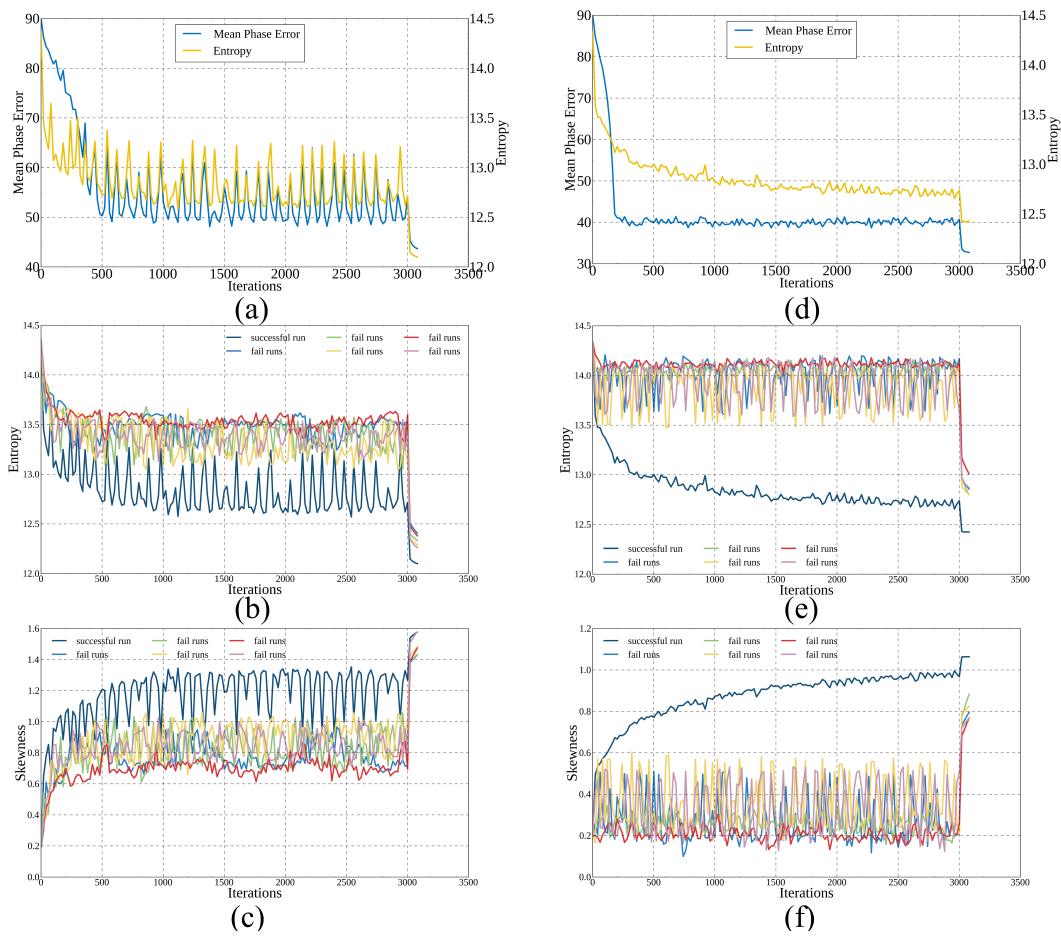


Figure S7 The trajectories of the mean phase error and entropy for a successful run. And the trajectories of the mean phase error and skewness. There are five non-converging curves and the converging curves are in dark blue. (a-c) 1BOT (d-f) 1KOA.

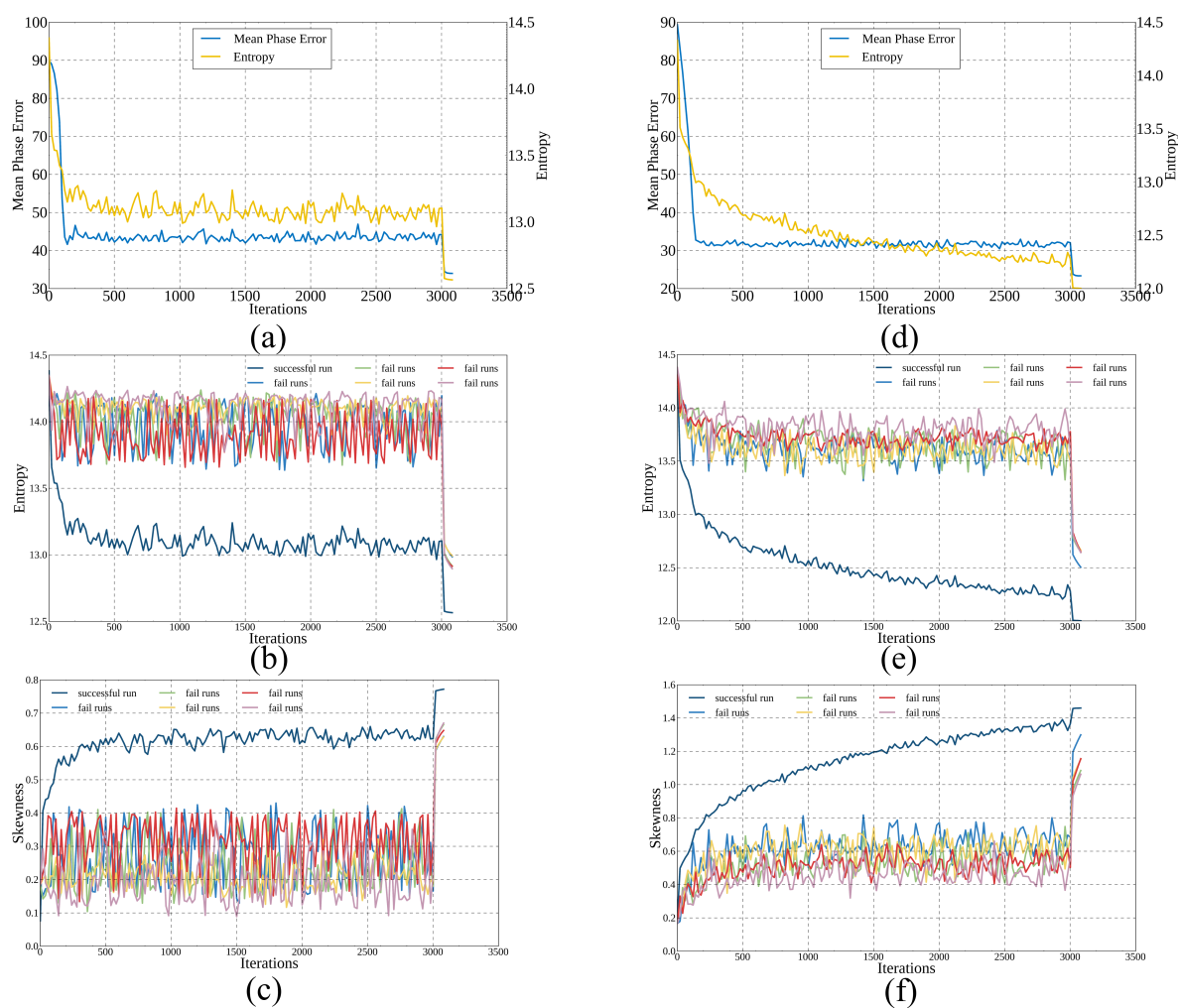


Figure S8 The trajectories of the mean phase error and entropy for a successful run. And the trajectories of the mean phase error and skewness. There are five non-converging curves and the converging curves are in dark blue. (a-c) 4AVT (d-f) 7STQ.

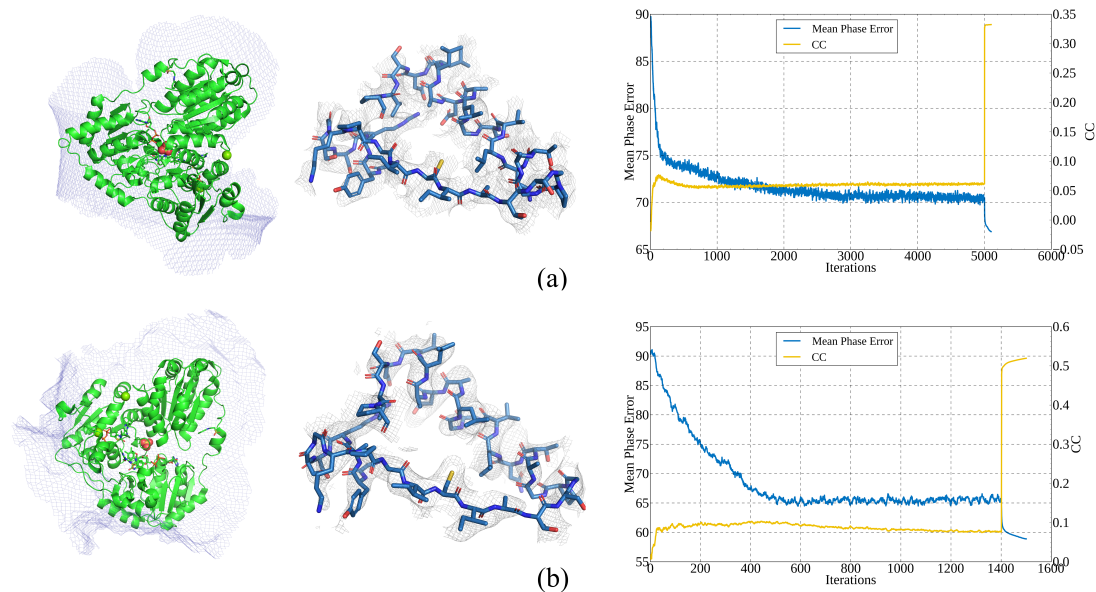


Figure S9 Experimental validation result of protein with PDB code 7STQ. (a) The randomly generated envelope, recovered electron density map and convergence plot after the initial iterative phase retrieval procedure. (b) The improved envelope, electron density map and convergence plot after another cycle of phasing-dm procedure. The electron density map is contoured at 1.0σ with the atomic model superimposed.

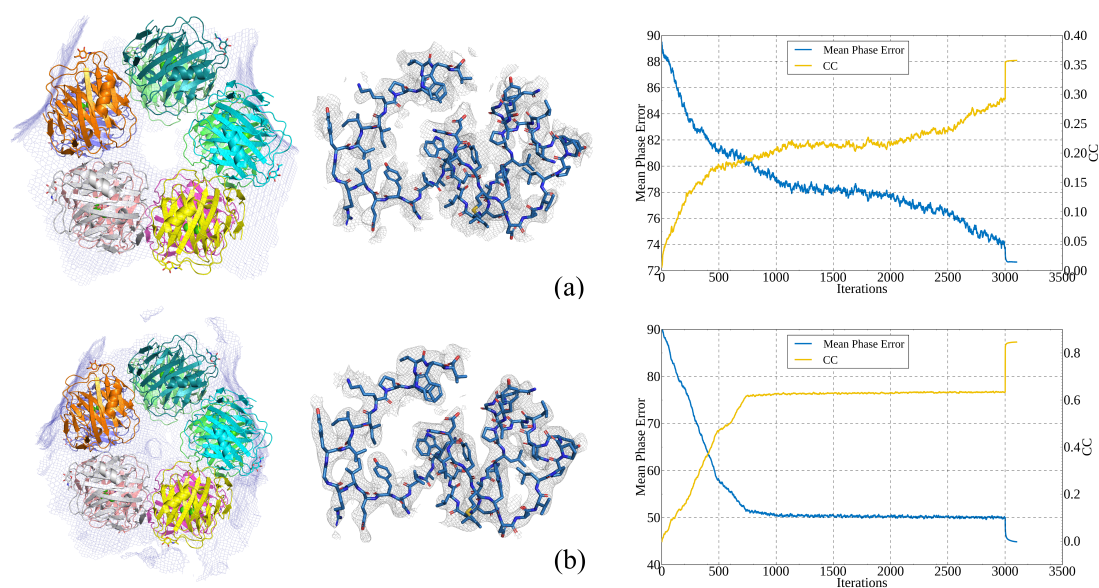


Figure S10 Experimental validation result of protein with PDB code 4AVT. (a) The randomly generated envelope, recovered electron density map and convergence plot after the initial iterative phase retrieval procedure. (b) The improved envelope, electron density map and convergence plot after another cycle of phasing-dm procedure. The electron density map is contoured at 1.0σ with the atomic model superimposed.

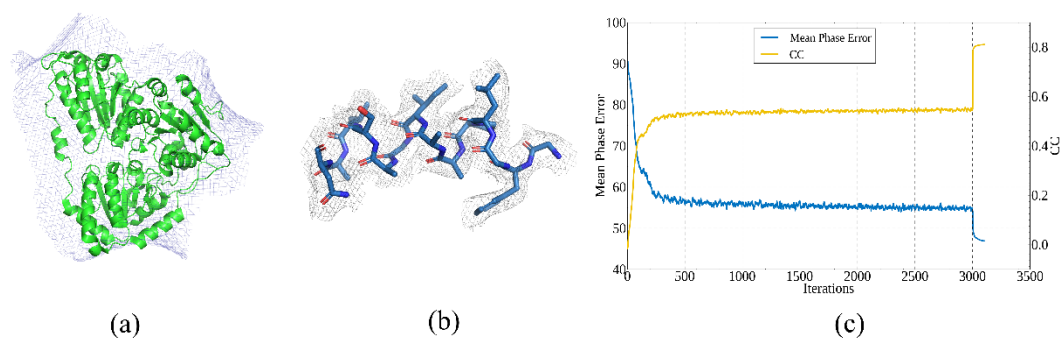


Figure S11 Experimental validation result of protein with PDB code 3E9Y. (a) The randomly generated envelope, recovered electron density map and (c) convergence plot after the initial iterative phase retrieval procedure. The electron density map is contoured at 1.0σ with the atomic model superimposed.