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Supporting information for article:

Molecular-replacement phasing using predicted protein structures from *AWSEM-Suite*

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S1 Electron density map comparison of 6 structure prediction targets corresponding in Figure 3.

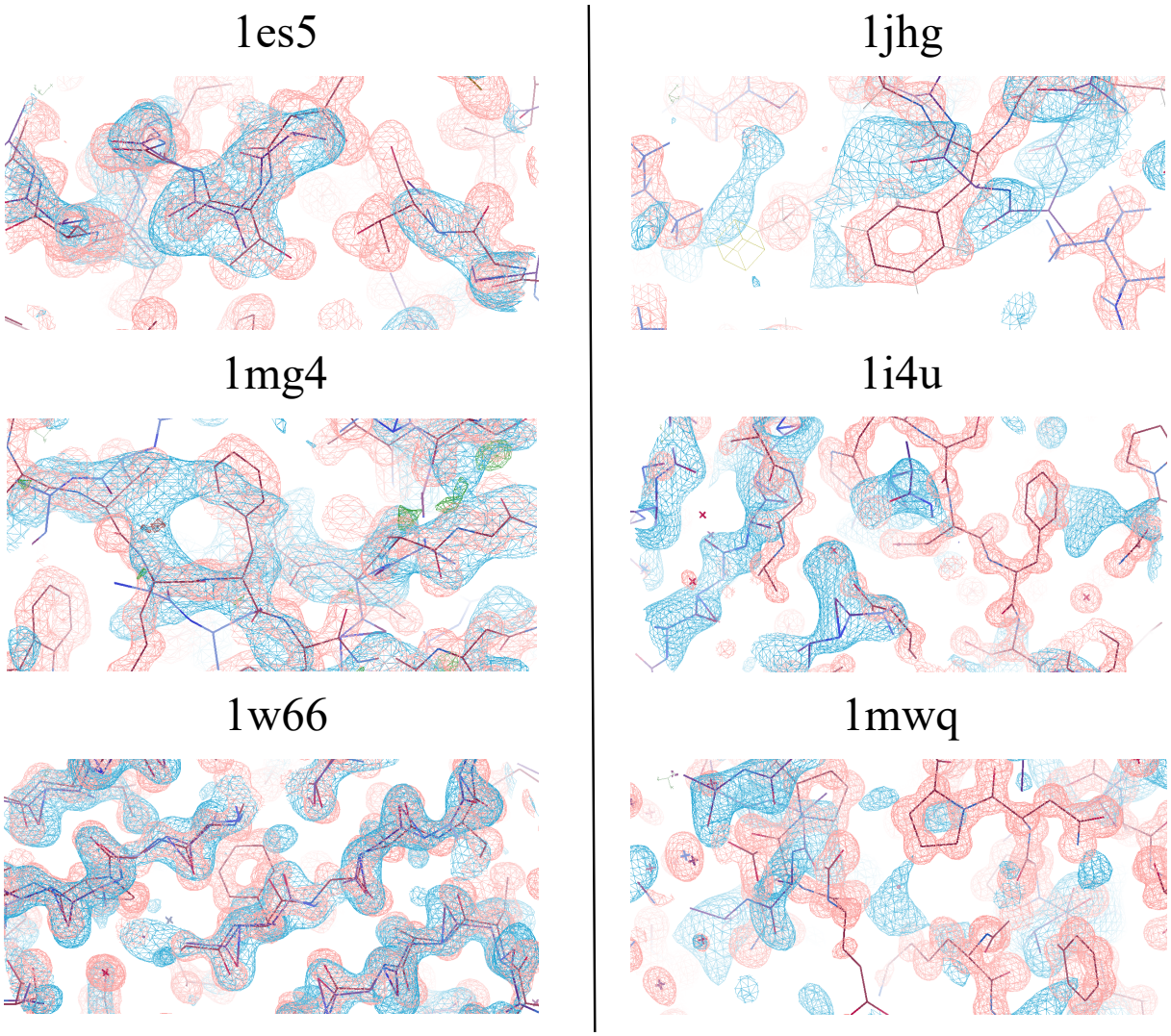


Figure S1: The electron density maps of 6 structure prediction targets corresponding in Figure 3. The red structure and density map show the data from crystal structure while the blue structure and density map show the data from AWSEM-Suite predicted structure after Phaser placement.

S2 Evaluation the quality of molecular replacement with other quantities.

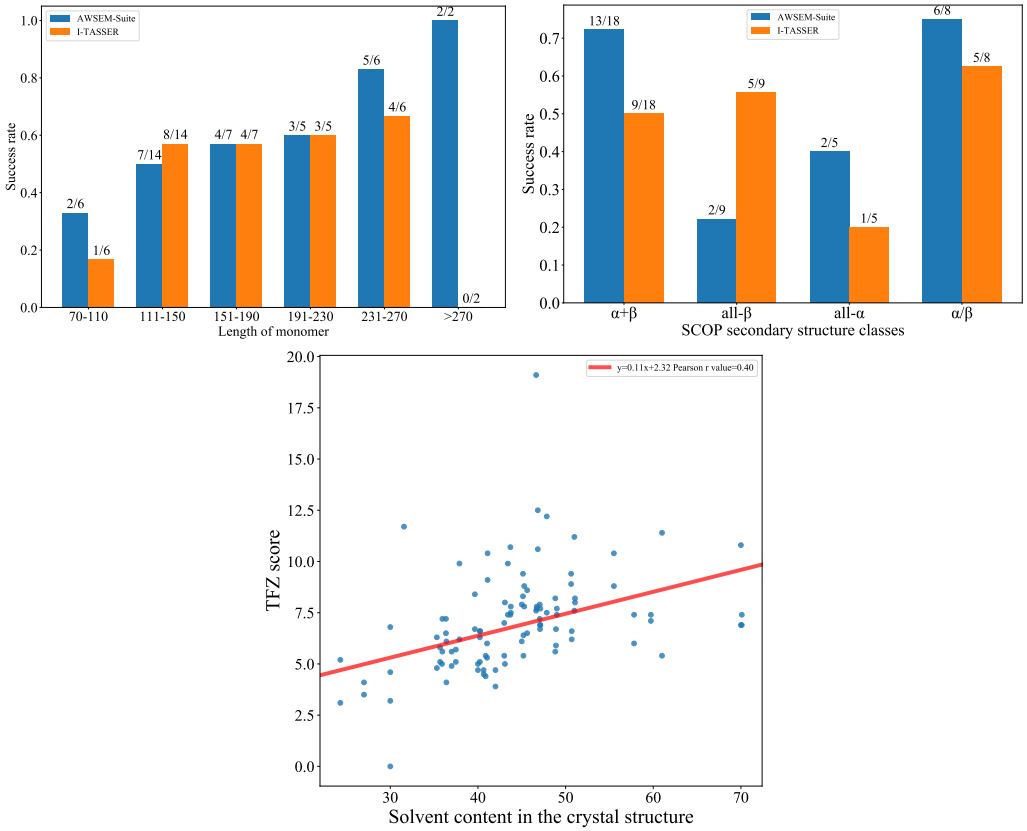


Figure S2: Evaluation the quality of molecular replacement with other quantities. The success rate of AWSEM-Suite as a function of the monomer length and secondary structure classes are plotted in the top and middle. AWSEM-Suite and I-TASSER are shown in blue and orange colors. The bottom is the TFZ score as a function of solvent content of the crystal structure (one outlier 1w66 is excluded). A strong correlation (Pearson r-value equals 0.4) is founded.

S3 Differential frustration analysis of 1tu9 and 1mwq.

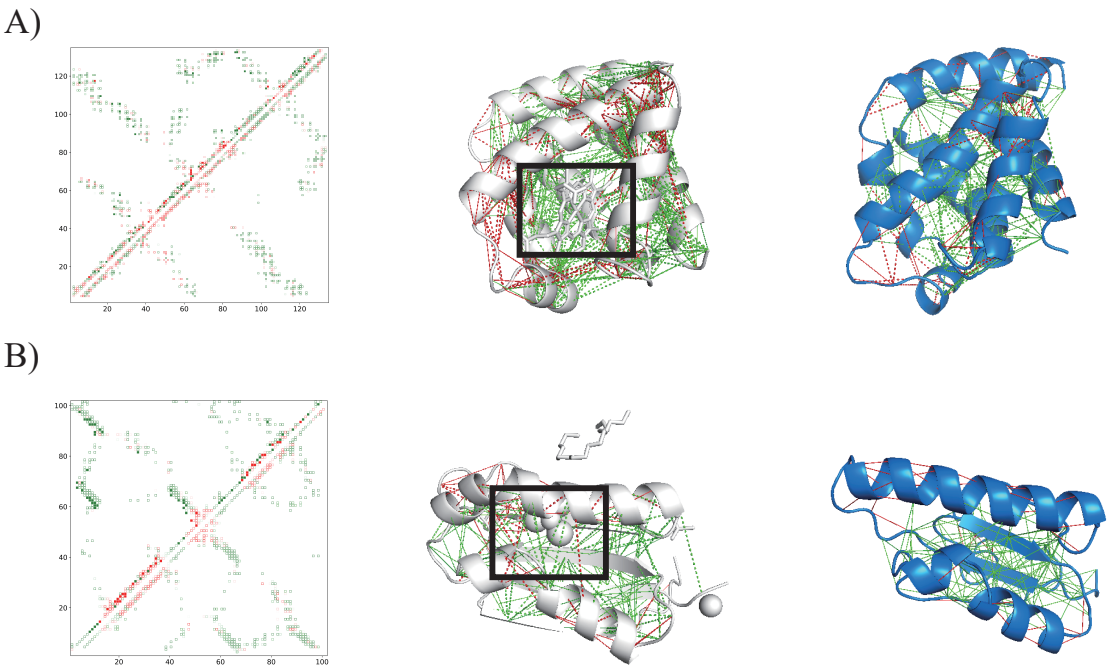
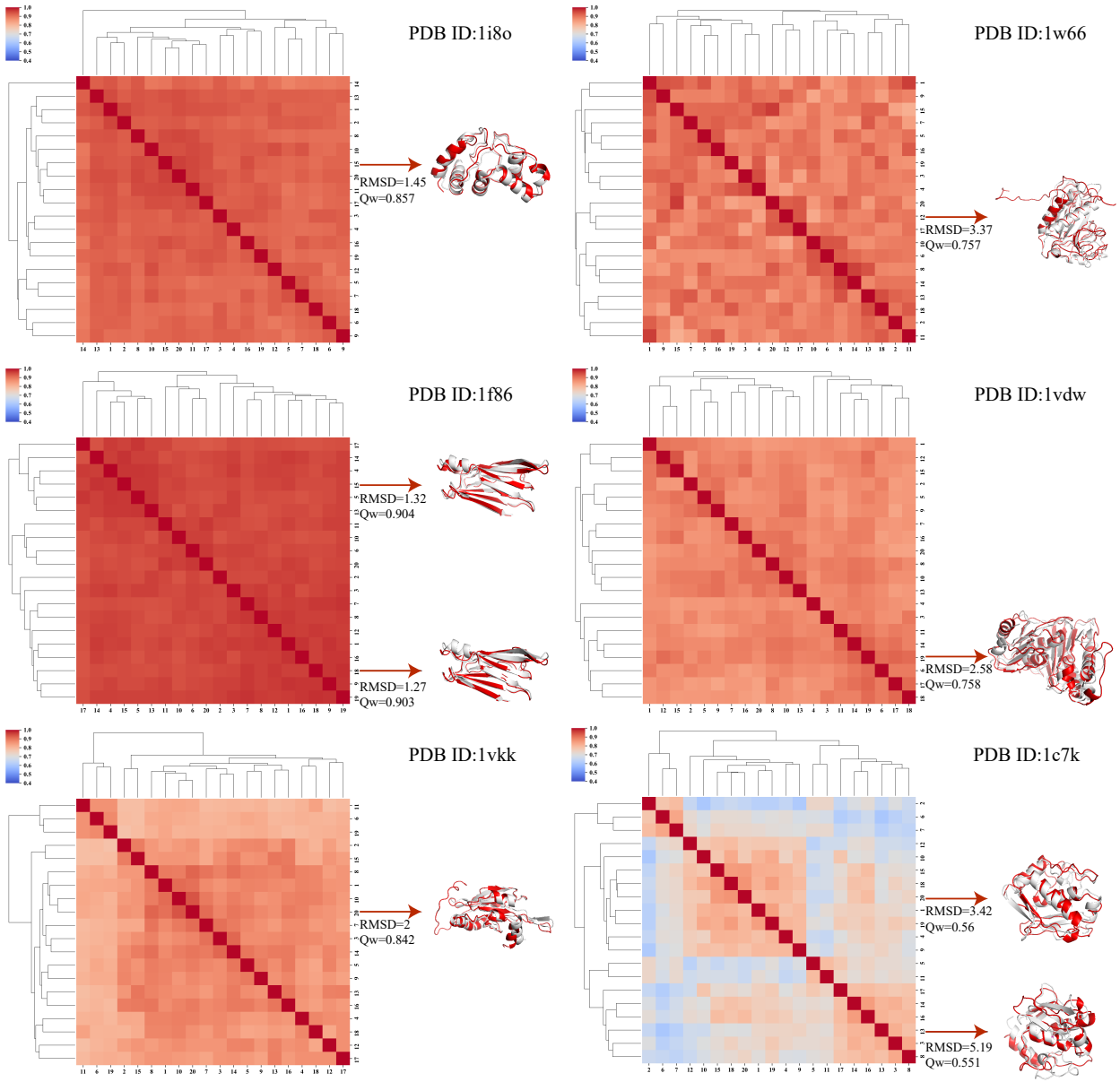
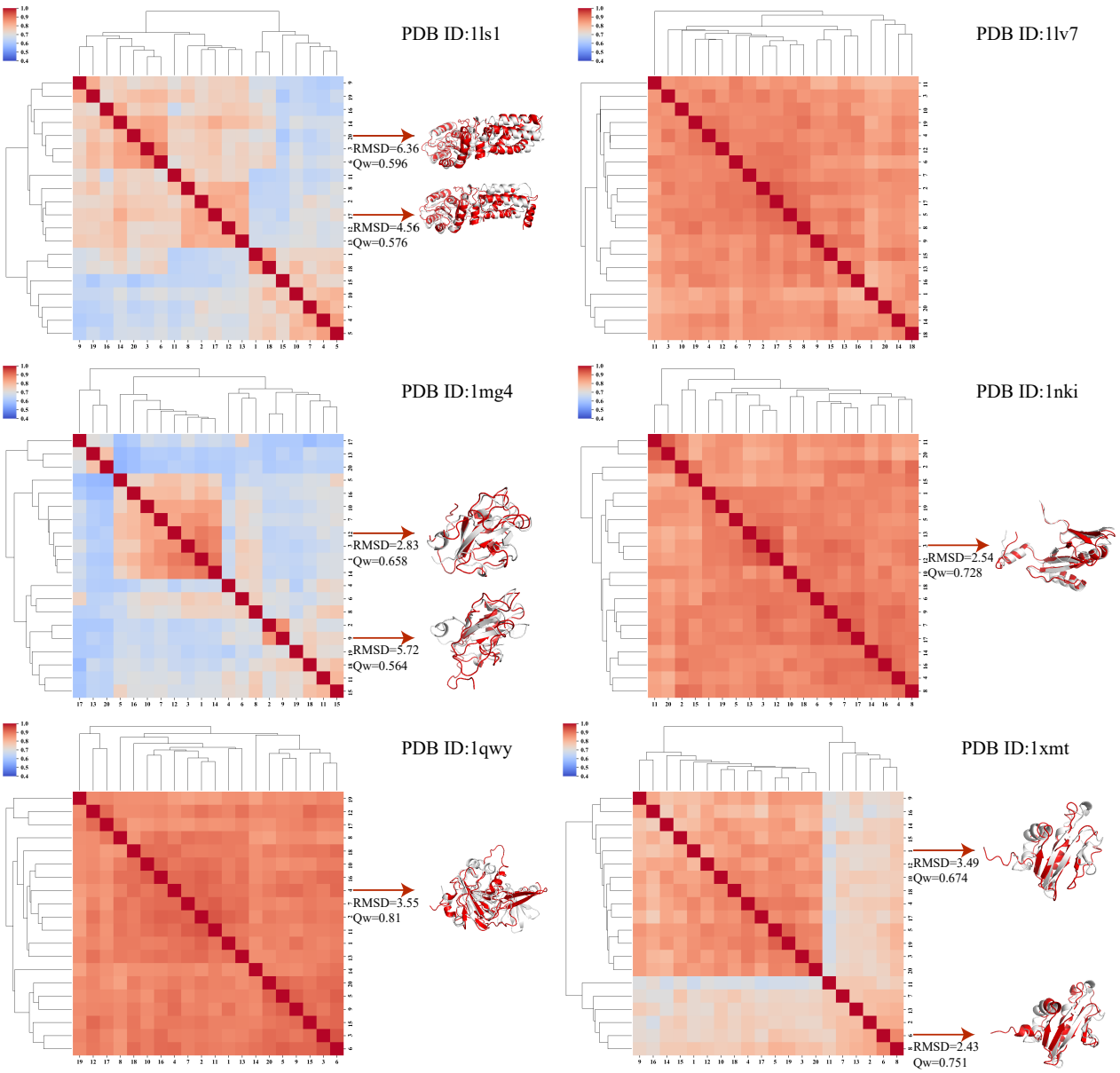


Figure S3: Differential frustration analysis of 1tu9 and 1mwq. The frustration contact maps in the left are comparing the residue frustration of the crystal structure (upper left) and the submitted structure (lower right). The color shows the range of frustration for each residue and the differential part of frustration analysis between two sturctures are plotted in green or red solid square (red solid square represents the residue interaction is a highly frustrated interaction in predicted structure but not in the crystal while the green square represents the a minimally frustration interaction is presents in predicted structure but not crystal). The structures on the right shows the frustration pattern of crystal (white) and predicted structure (blue). The position of cofactors are highlighted black box.

S4 Clustermap for different targets.

Figure S4: Clustermap for different targets. Among these targets, 1i8o, 1w66, 1f86, 1vdw, 1vkk are easy targets. The remaining solvable cases are all belong to hard targets.

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Qw=0.564
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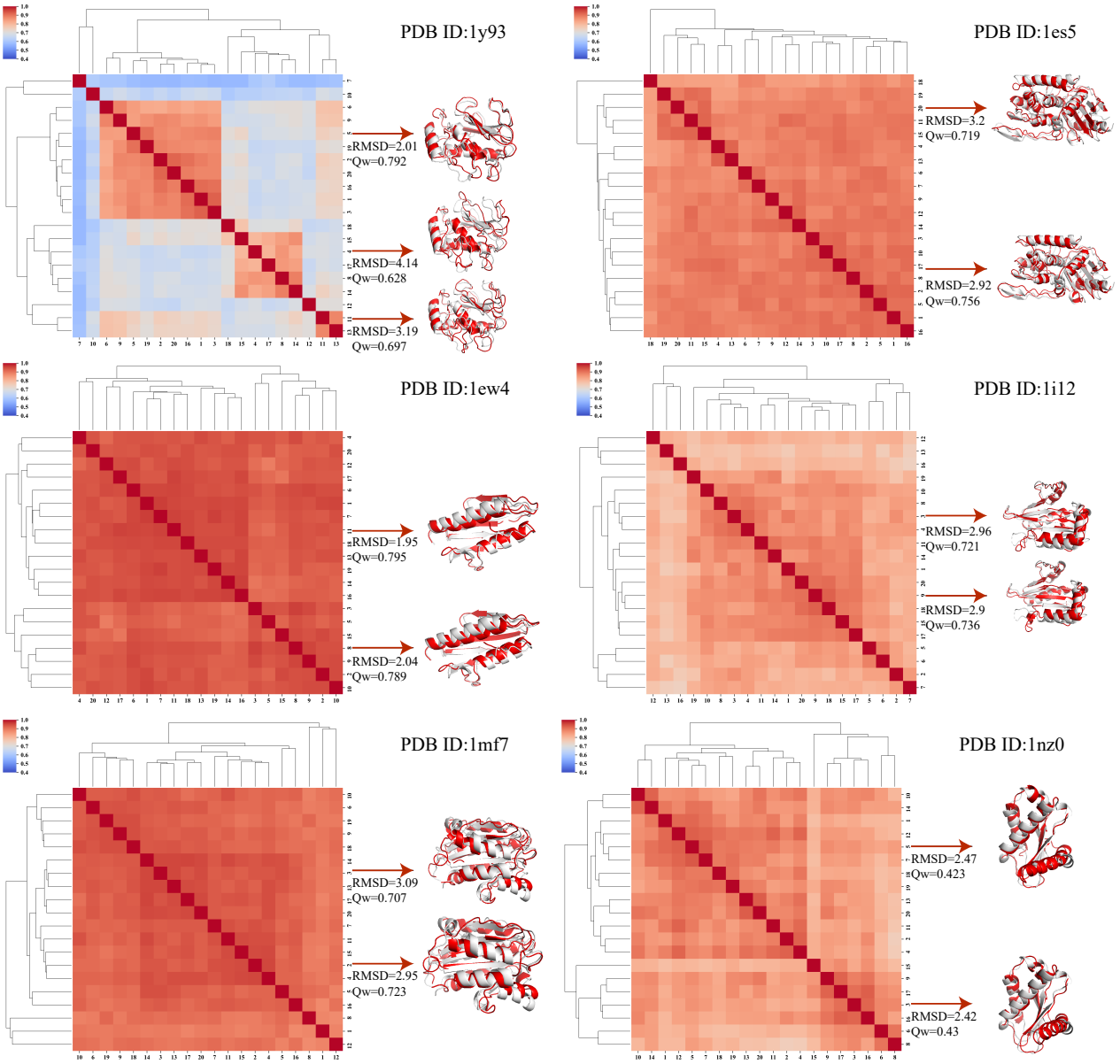
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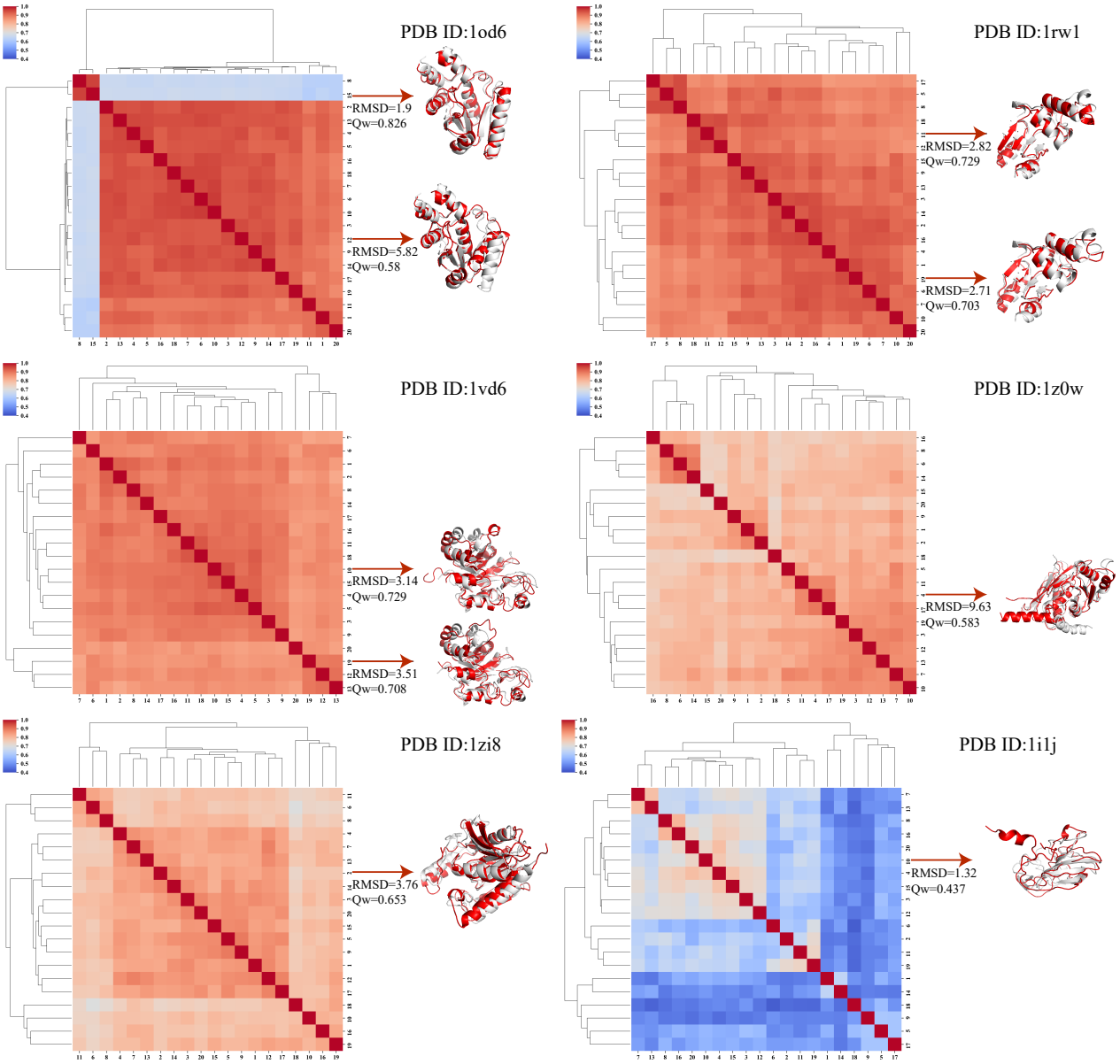
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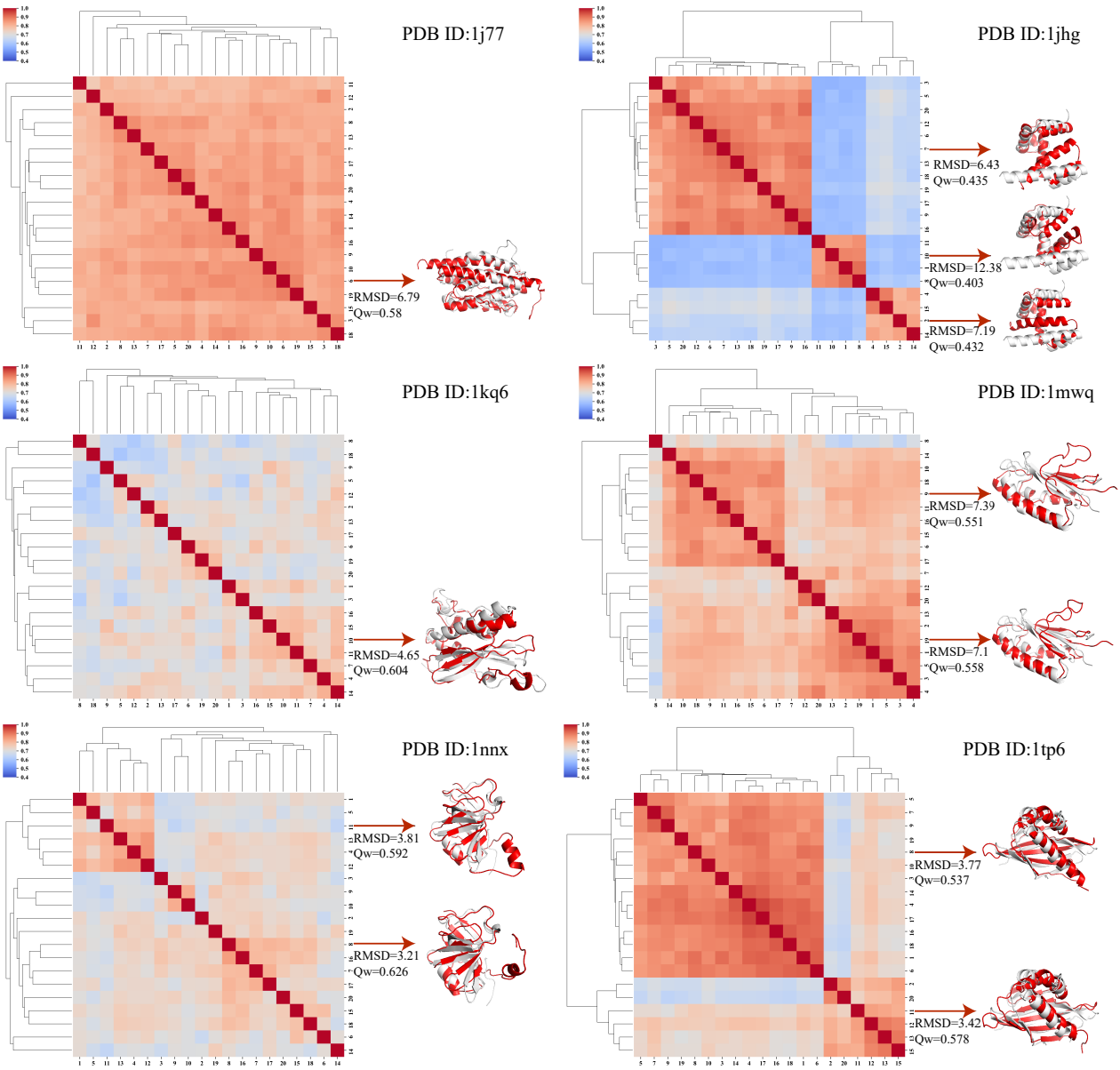
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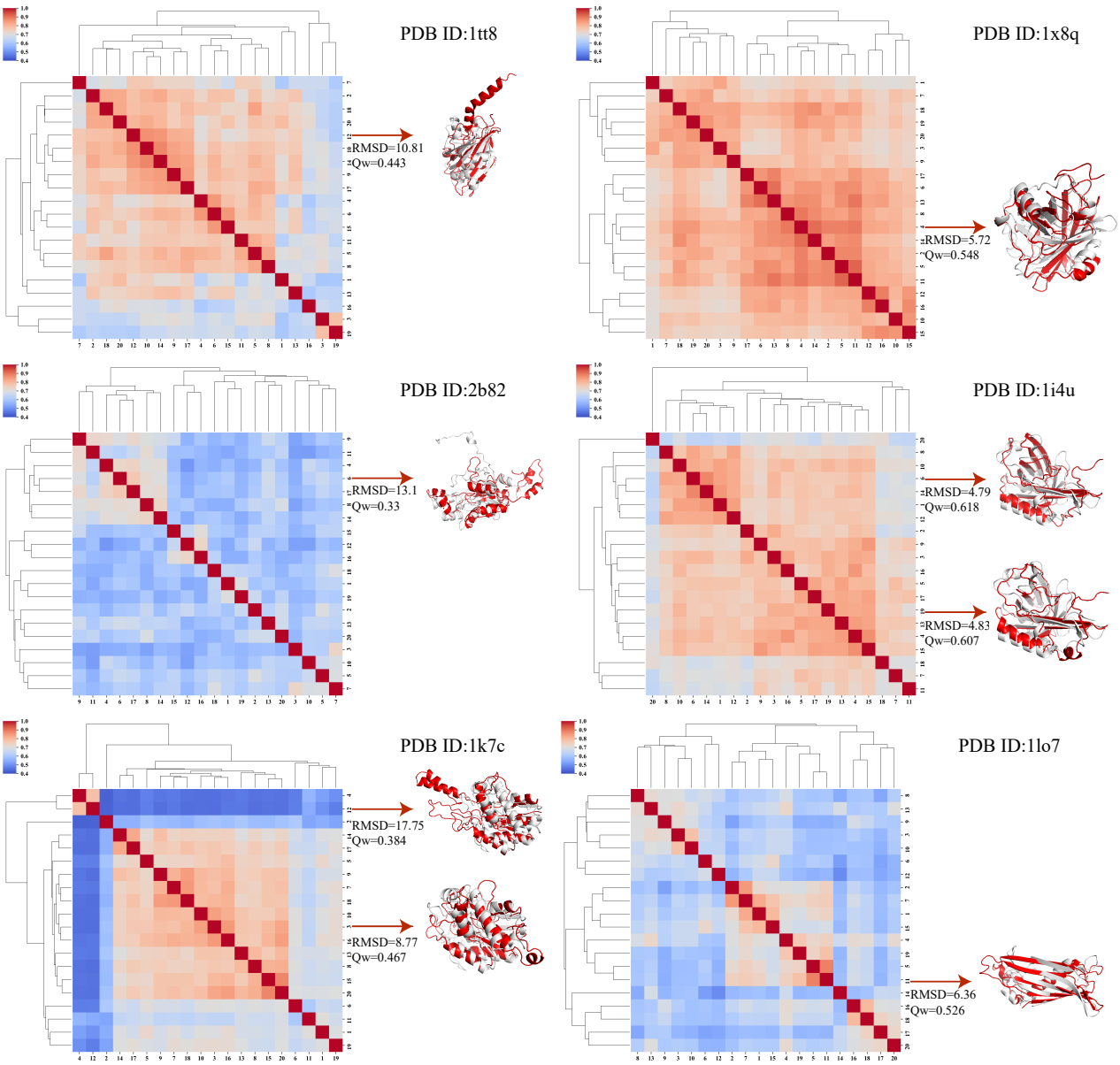
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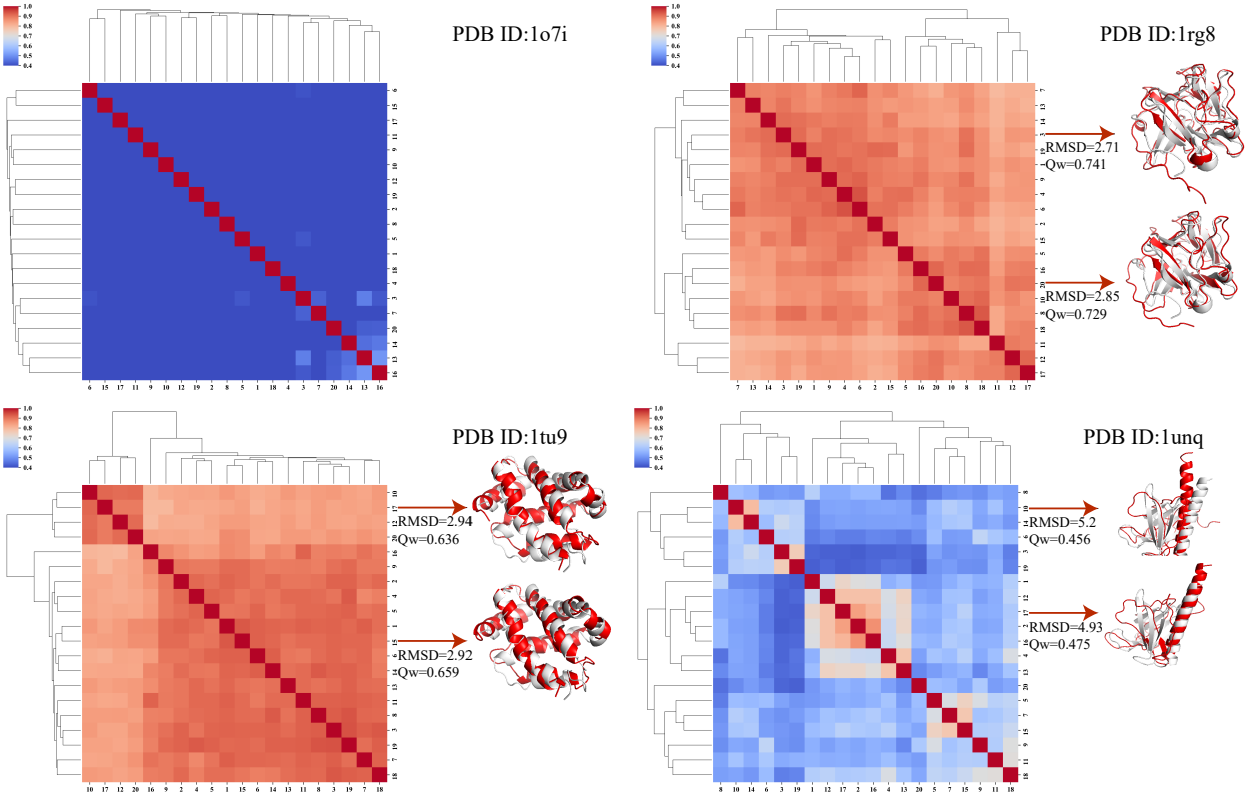
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S5 Map CC score for four cases that pre-aligned search of AWSEM-Suite predicted model can solve.

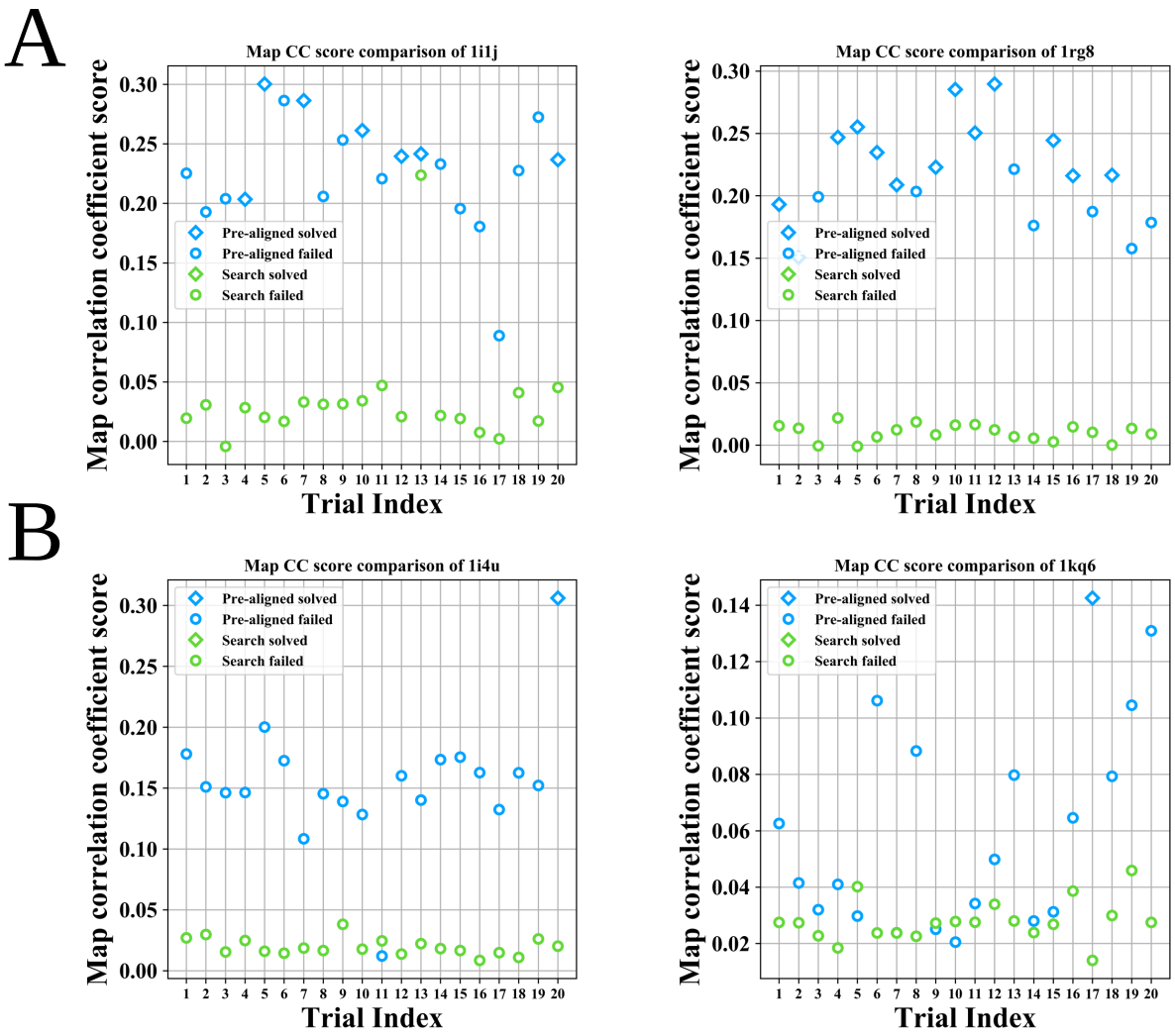

Figure S5: Map-CC for four cases that pre-aligned search of AWSEM-Suite predicted model can solve. For the panel A, most trials of these two cases are successful that indicate the searching procedure is not optimal. For the panel B, only one trial leads to the successful solution but the molecular replacement program are all failed to find.