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Supplemental Information

Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution

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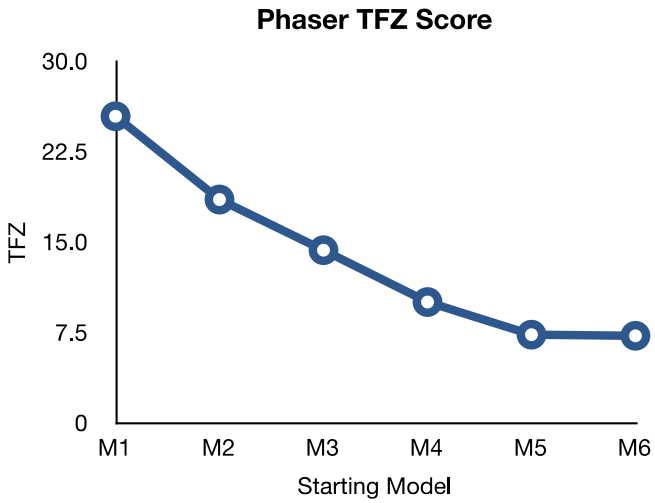
Table S1. The required X-ray resolution (determinacy point) depends on the number of degrees of freedom and the solvent fraction (related to Figure 1).

a



b

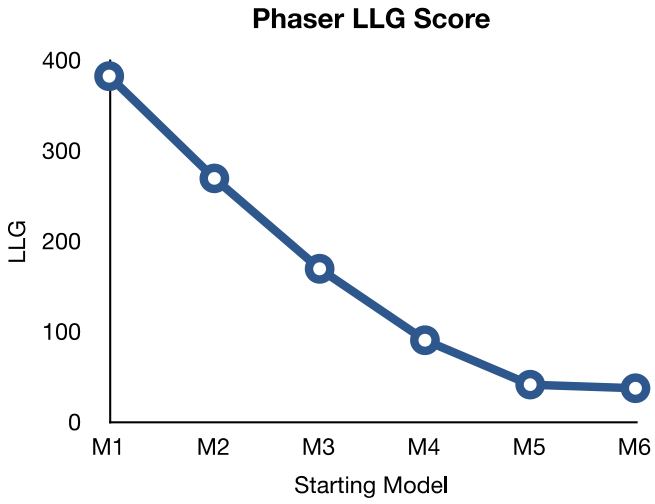


Figure S1. Molecular replacement results using the 7.4 Å diffraction data of PSI with models M1 through M6 (related to Figure 1). (**a**) Translation function Z-score (TFZ) for models M1-M6. (**b**) Corresponding log-likelihood gain (LLG) of the translation function solution. The molecular replacement was carried out with Phaser (McCoy et al., 2007).

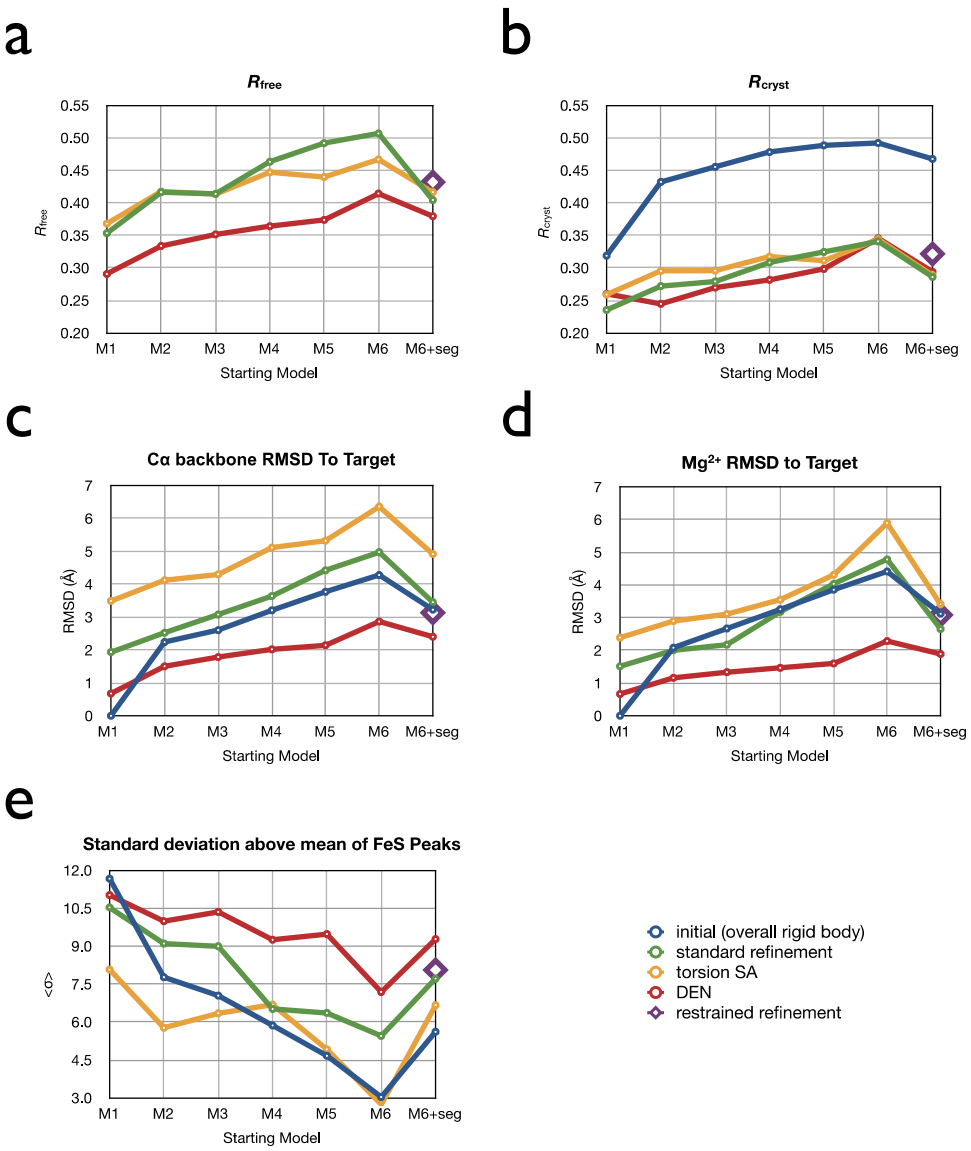
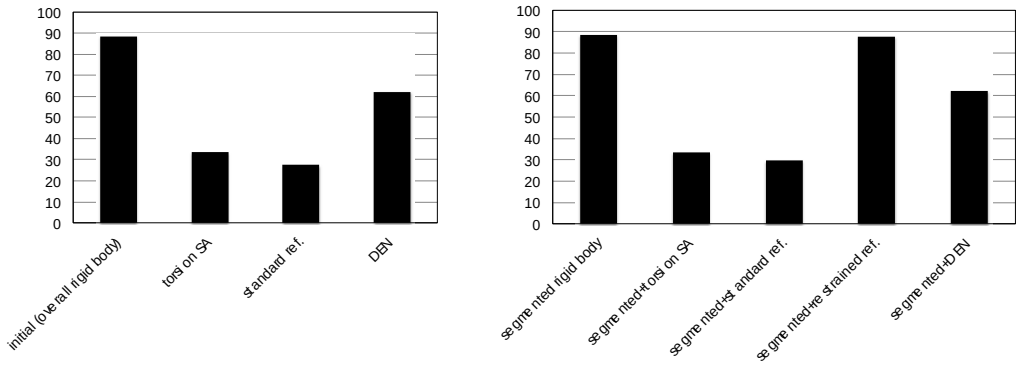


Figure S2. Refinements against the 7.4 Å diffraction data of PSI starting from models M1 to M6 (related to Figure 2). In addition, for model M6, the structure was first subjected to segmented rigid body refinement ("M6+seg"). The refinement methods are indicated in the legend. (**a**) R_{free} of the refined models. (**b**) R_{cryst} (computed for the working set) of the refined models. (**c**) Cα backbone RMSD between the refined models and the 2.5 Å structure of PSI (PDB ID 1jb0). (**d**) RMSD of the Mg^{2+} ions of the 96 chlorophyll cofactors between the refined models and the 2.5 Å structure of PSI. (**e**) <σ>, the average Z-Score (average number of standard deviations above the mean) of the three difference peaks in mF_o-DF_c maps for the iron-sulfur clusters that were omitted during the refinements. Details of the refinement methods, RMSD calculation, and difference peak calculations are described in Experimental Procedures. Note that R_{free} is highly correlated with R_{cryst} for rigid body refinement since only a few parameters are refined which results in potential bias of the test set towards the working set (Brunger, 1993). Thus, R_{free} is not shown for the rigid body refinement in panel **a**.



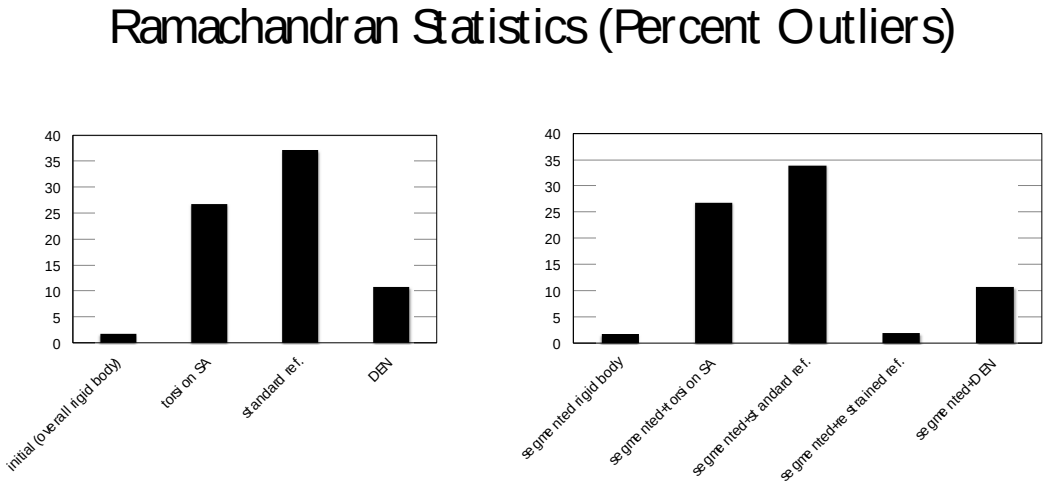


Figure S3. Ramachandran statistics (percent favored and percent outliers) for specified refinements starting from model M6 against the 7.4 Å diffraction data of PSI (related to Figure 3). Molprobity (Chen et al., 2010) was used to calculate the Ramachandran statistics.

Table S1. The required X-ray resolution (determinacy point) depends on the number of degrees of freedom and the solvent fraction (related to Figure 1)[1]

Degrees of Freedom & N/N_{res}		***S* (Solvent Volume Fraction)**		
		0.5	**0.6**	**0.7**
All atoms with H atoms	**48**	2.3 Å	2.5 Å	2.8 Å
All atoms no H atoms	**24**	2.9 Å	3.2 Å	3.5 Å
All (Φ,Ψ,χ) torsions	**4**	5.3 Å	5.8 Å	6.3 Å
All (Φ,Ψ) torsions	**2**	6.7 Å	7.3 Å	8.0 Å
All (α) torsions	**1**	8.5 Å	9.13 Å	10.1 Å

[1]Number of X-ray reflections, $N=2\pi V/3Zd^3$, where V is the unit cell volume

$V = ZV_{prot}/(1-S)$,

Z is the symmetry redundancy, d is resolution and S is the solvent volume fraction. The protein volume,

$V_{prot} = N_{res}*(30/18)*0.73*119 = 145N_{res}$,

using a water volume of 30 A^3 per 18 Dalton at a density of 1 g/ml, a protein specific volume of 0.73 ml/g and average residue mass of 119 D. Substituting for V in the expression for N gives:

$N =2\pi ZN_{res}145/(1-S)/(3Zd^3) =(2\pi 145/3)N_{res}/((1-S)d^3) =304N_{res}/((1-S)d^3)$

or

$N/N_{res} =304/(1-S)d^3$.

Solve for d in terms of (N/N_{res}) and S to give

$d =[304/((1-S)*(N/N_{res})]^{1/3}$.

The number of degrees of freedom per residue is approximately 48 for all atoms including hydrogen atoms, 24 for just heavy atoms, 4 for all single bond torsion angles (Φ,Ψ,χ), 2 for just main chain (Φ,Ψ) torsion angles, and 1 for main chain α angles.