

Supplemental Table I. Crystallographic Data and Refinement Statistics

PDB ID	Native 1Z5S
Source	APS 31ID
Wavelength (Å)	0.9793
Resolution Limits (Å)	50-3.0
Space Group	P3 <sub>2</sub> 21
Unit Cell (Å) a, b, c, α, β, γ	157.1, 157.1, 59.6, 90, 90, 120
Number of observations	147869
Number of reflections	16464
Completeness (%)	97.0 (91.8)
Mean I/σI	15.1 (2.1)
R-merge on I <sup>a</sup>	7.5 (46.4)
Cut-off criteria I/σI	0
<u>Refinement Statistics</u>	
Resolution Limits (Å)	30-3.0
Number of reflections	16461
Completeness (%)	96.5 (86.2)
Cutoff Criteria I/σI	0
Protein/water atoms	3564/28
Rcryst <sup>b</sup>	0.247 (0.425)
Rfree (5% of data)	0.290 (0.432)
Bonds (Å) <sup>c</sup>	0.006
Angles (°) <sup>c</sup>	1.2
Bfactor (mc/sc in Å <sup>2</sup> ) <sup>c</sup>	2.27/2.80

a.  $R_{merge} = \frac{\sum hkl \sum i |I(hkl)_i - \langle I(hkl) \rangle|}{\sum hkl \sum i \langle I(hkl)_i \rangle}$ .

b.  $R_{cryst} = \frac{\sum hkl |F_o(hkl) - F_c(hkl)|}{\sum hkl |F_o(hkl)|}$ , where  $F_o$  and  $F_c$  are observed and calculated structure factors, respectively.

c. Values indicate root-mean-square deviations in bond lengths, bond angles, and Bfactors of bonded atoms.

Parentheses indicate statistics for the high-resolution data bin for x-ray and refinement data.

Data were processed using DENZO, SCALEPACK<sup>1</sup>, and CCP4<sup>2</sup>. The structure was solved by molecular replacement using CCP4<sup>2</sup>. The atomic model was built using O<sup>3</sup> and refined using CNS<sup>4</sup>.

1. Otwinowski, Z. & Minor, W. Processing of X-ray Diffraction Data Collected in Oscillation Mode. *Methods in Enzymology* **276**, 307-326 (1997).

2. Collaborative Computational Project. The CCP4 suite: programs for protein crystallography. *Acta Crystallography* **D50**, 760-763 (1994).

3. Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models. *Acta Crystallogr. A* **47 (Pt 2)**, 110-119 (1991).

4. Brunger, A. T. *et al.* Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallogr. D. Biol. Crystallogr.* **54 (Pt 5)**, 905-921 (1998).