**SUPPLEMENTARY MATERIALS**

1. Figure S1. Representative electron density with experimental and model phases

2. Figure S2. Details of crystal contact giving clashes

3. Figure S3. Ramachandran Plot.

**SUPPLEMENTARY FIGURE S1**

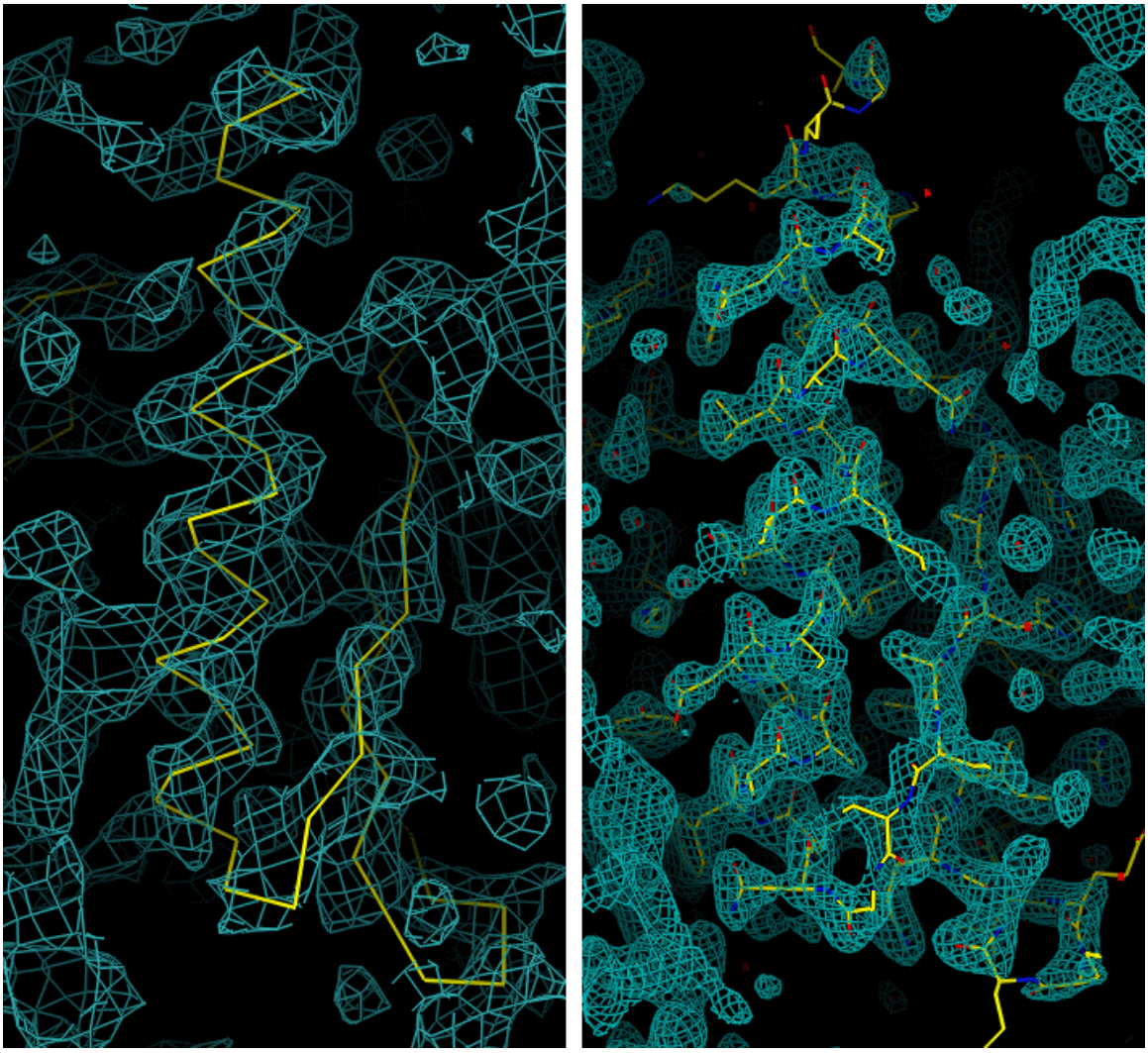

**Figure S1** Sample density containing experimental phases. *Left*: $F_{obs}$-PHIB-$F_{om}$ map, 4.0Å (contoured 1σ). *Right*: phases from the final, refined model. $2F_o$-$F_c$, 1.6Å (contoured $0.5e^-/Å^3$ = 1.29σ). Helix 2 and strand 5 are visible. The final model is shown as a C-α trace (left) and stick figure (right).

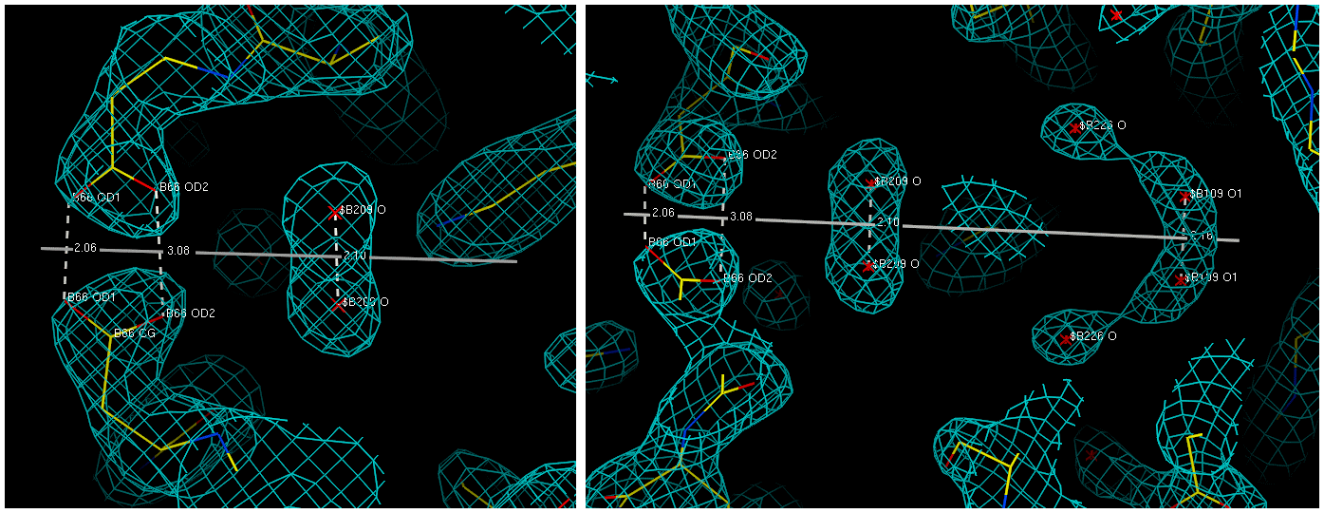


Figure S2. Close contacts with symmetry mate. A. view optimized to show interaction between Asp66 in chain B and its symmetry mate. The contact involving water 209 is also visible. B. All three contacts including "unknown ligand" B109 (rightmost crescent-shapped density). The near-horizontal gray lines in both figures approximate the crystallographic 2-fold axis relating the clashing pairs of atoms.

**SUPPLEMENTARY FIGURE S3**

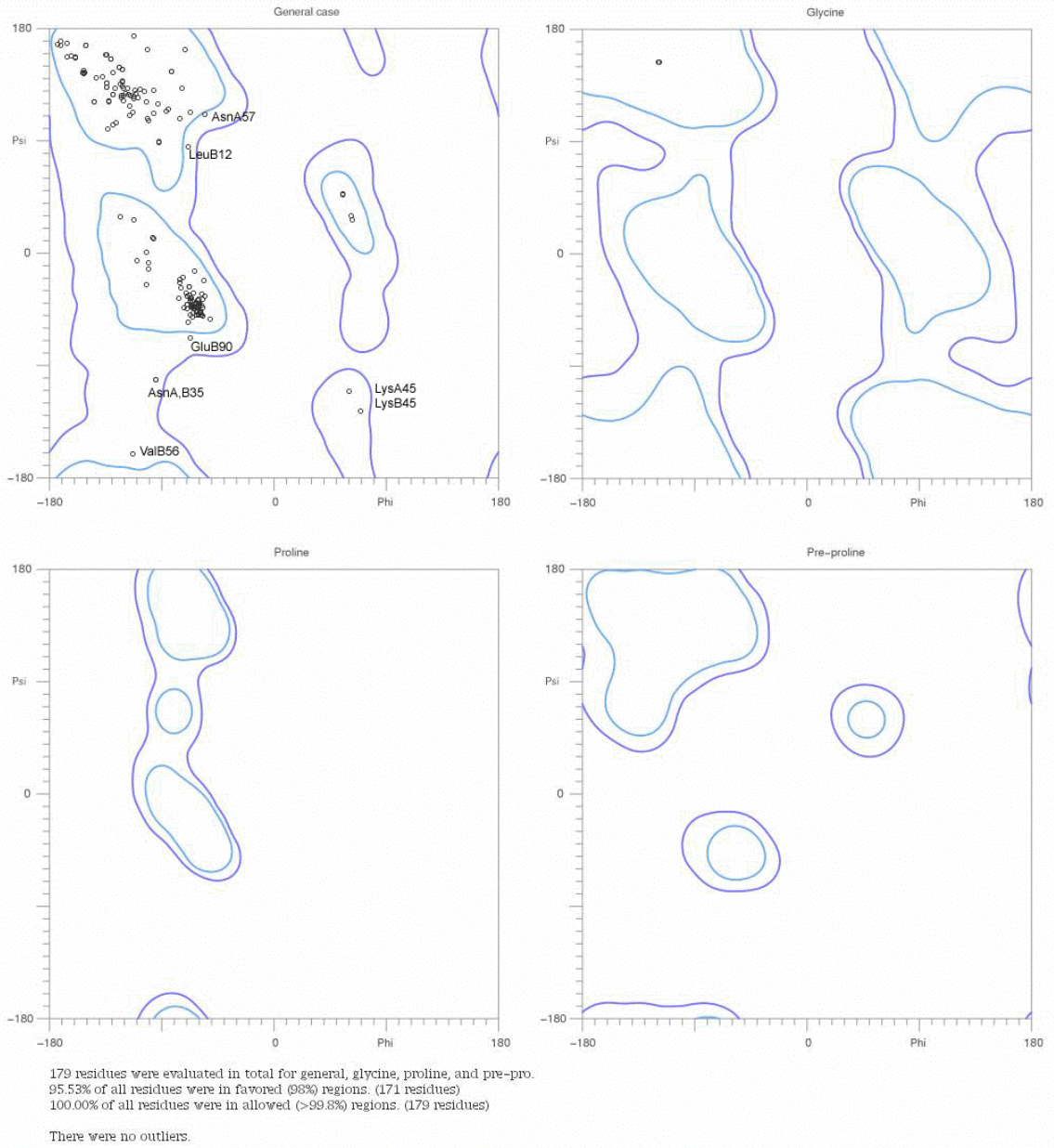


Figure S3. Ramachandran plot for final structure. There are eight residues outside the most favorable zone (Asn35 and Lys45 in both chains, Asn57 in chain A, and Lys12, ValB56 and Glu90 in Chain B) and no residues in the disallowed zone. There are two glycine residues (Gly 7 in each chain) and no proline residues.