## Structural insight into the substrate selectivity of the *Erwinia chrysanthemi* Lasparaginase

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## Supplementary Data



Supplementary Figure S1. ErA-ASP complex simulated annealing omit maps of key residues. Omit density for the ligand ASP as seen in A. Protomer B (light blue). B. Protomer B (light pink). C. Protomer D (light yellow). Omit density for Thr15 as seen in D. Protomer B (light blue). E. Protomer B (light pink). F. Protomer D (light yellow). Map used is a simulated annealing omit map, contoured at 2.5 sigma, where the ligand ASP was not included in the model, and Thr15 was mutated to a glycine, for the simulated annealing step.



**Supplementary Figure S2.** *ErA*-GLU complex simulated annealing omit maps of key residues. Omit density for the ligand GLU as seen in **A.** Protomer B (dark blue). **B.** Protomer C (dark pink). Omit density for Thr15 as seen in **C.** Protomer B (dark blue). **D.** Protomer C (dark pink). Map used is a simulated annealing omit map, contoured at 2.5 sigma, where the ligand GLU was not included in the model, and Thr15 was mutated to a glycine, for the simulated annealing step.



Supplementary Figure S3. Simulated annealing omit map for *ErA*-GLU, showing the N-terminal residues (Ser19 to Ala33) of Protomer D. Presented as a stereo figure, the map is a 2Fo-Fc SA omit map contoured at 0.5 sigma.



Supplementary Figure S4. Conserved Gly14 provides the required main chain flexibility for the change in conformation of Thr15. Distances between corresponding main chain atoms (gray arrows) are shown in Angstroms.



**Supplementary Figure S5. Plot of average residue B-factor versus residue number.** Note the very similar B-factor values for the *Erw*-ASP and *Erw*-GLU structures (shown is the analysis for the respective protomer D), but much higher B-factor values for the N-terminal loop region for the *Erw*-GLU complex. The N-terminal loop of protomer D of the *Erw*-GLU structure was modeled with a partial occupancy of 0.67; despite this fact the B-factors are higher than the corresponding *Erw*-ASP region, showcasing a less stabilized region.