

Supplementary Table S4: Data collection and refinement statistics.

| <i>V. cholerae</i> AspS | |
|---|--|
| Data collection | |
| Space group | <i>P</i> 2 ₁ 2 ₁ 2 |
| Cell dimensions | |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 34.16, 63.86, 47.54 |
| α , β , γ (°) | 90, 90, 90 |
| Resolution (Å) | 47.5-1.48 (1.56-1.48) ¹ |
| <i>R</i> _{sym} | 0.084 (0.851) |
| <i>I</i> / σ <i>I</i> | 16.2 (1.73) |
| Completeness (%) | 98.3 (89.0) |
| Redundancy | 7.2 (5.0) |
| Refinement | |
| Resolution (Å) | 47.5-1.48 |
| No. reflections (total/free) | 17689/907 |
| <i>R</i> _{work} / <i>R</i> _{free} | 0.155/0.176 (0.232/0.248) |
| No. atoms | |
| Protein | 830 |
| Ligand/ion | 15 |
| Water | 169 |
| <i>B</i> -factors | |
| Overall | 17.2 |
| Protein | 14.7 |
| Ligand/ion | 18.5 |
| Water | 29.6 |
| Wilson <i>B</i> | 20.1 |
| R.m.s. deviations | |
| Bond lengths (Å) | 0.013 |
| Bond angles (°) | 1.53 |
| Ramachandran distribution (%) ² | |
| Favored | 99.1 |
| Outliers | 0.0 |

¹Values in parentheses are for highest-resolution shell.

²Calculated using Molprobit.