

S1 Table. Crystallographic data collection and refinement statistics

| | ANDV L ₁₋₂₀₀ K127A anomalous | ANDV L ₁₋₂₀₀ K127A native |
|--|---|--------------------------------------|
| Data collection | | |
| Space group | P 42 ₁ 2 | P 42 ₁ 2 |
| Cell dimensions (Å/°) | a=b=82.9; c=79.3 α=β=γ=90° | a=b=82.9; c=79.3 α=β=γ=90° |
| Wavelength (Å) | 1.77 | 0.984 |
| Resolution range (Å) | 79.31 – 2.80 (2.87 – 2.80) | 79.31 – 2.40 (2.46 – 2.40) |
| Completeness (%) ¹ | 99.88 (100) | 99.3 (99.6) |
| Observed reflections | 93605 (18108) | 84120 (18266) |
| Unique reflections | 13170 (2446) | 20577 (4391) |
| Redundancy ¹ | 7.1 (7.4) | 4.1 (4.2) |
| R _{merge} (%) ¹ | 10.9 (126.9) | 4.9 (98.0) |
| Mean I/σ ¹ | 14.2 (1.8) | 19.3 (2.1) |
| Wilson B-factor | 59.74 | 52.16 |
| Refinement statistics | | |
| R _{work} (%) / R _{free} (%) ² | | 20.8/26.2 (38.2/42.5) |
| Average B-factor (Å ²) | | 72.4 |
| Protein | | 72.6 |
| Ligand | | 74.0 |
| Solvent | | 67.7 |
| Number of atoms | | 1672 |
| Protein | | 1617 |
| Ligand | | 12 |
| Water molecules | | 42 |
| RMSD bond lengths | | 0.01 |
| RMSD bond angles | | 1.44 |
| Ramachandran favored (%) | | 93 |
| Ramachandran outliers (%) | | 0 |
| PDB ID | | 5HSB |

¹ Values in parentheses are for the highest resolution shell.

² R_{free} is the cross-validation R factor for 10% of reflections against which the model was not refined.