

Table S1: UNC119 crystallographic data and refinement statistics

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|--|---|---|
| Data | | |
| Crystal | HR3066a ^a | Au10pe |
| Space Group | P2 ₁ 2 ₁ 2 ₁ | P2 ₁ 2 ₁ 2 ₁ |
| Unit Cell Dimensions | a=77.89, b= 79.56, c=189.72 | a=78.55, b=79.71 , c=189.59 |
| Resolution (Å) | 50.0 – 1.95 | 30.0 – 2.00 |
| Resolution (Å) (high-resolution shell) | (2.02 – 1.95) | (2.07 – 2.00) |
| # Reflections measured | 1,169,802 | 1,252,665 |
| # Unique reflections | 166,290 ^a | 82,342 |
| Redundancy | 7.0 | 15.2 |
| Completeness (%) | 99.6 (100) | 100 (100) |
| <I/σ(I)> | 26 (2.9) | 11 (2.5) |
| Mosaicity (°) | 0.37 | 1.1 |
| Rsym ^b | 0.088 (0.537) | 0.116 (0.701) |
| | | |
| Refinement | | |
| Resolution (Å) | 40.51 – 1.95 | 29.37 – 1.99 |
| Resolution (Å) – (high-resolution shell) | (1.97 – 1.95) | (2.04 – 1.99) |
| # Reflections used for refinement | 165,606 ^a | 78,089 |
| # Reflections in Rfree set (%) | 8,332 (5.0) | 4,139 (5.3) |
| R ^c | 0.191 (0.247) | 0.200 (0.226) |
| Rfree ^d | 0.214 (0.251) | 0.250 (0.276) |
| RMSD: bonds (Å) / angles (°) | 0.005 / 1.3 | 0.012 / 1.304 |
| (Å ²): Tα peptide residues / # atoms | N/A | 41 / 268 |
| (Å ²): UNC119 only / # atoms | 33 / 8,265 | 29 / 8,299 |
| (Å ²): water molecules / # water | 41 / 803 | 39 / 793 |
| φ/ψ most favored (%) | 99 | 97 |

Values in parenthesis refer to data in the high resolution shell.

^a Friedel pairs were used in phasing and refining HR3066a.

^b Rsym = $\sum |I - \langle I \rangle| / \sum I$ where I is the intensity of an individual measurement and $\langle I \rangle$ is the corresponding mean value.

^c R = $\sum ||F_o| - |F_c|| / \sum |F_o|$, where |F_o| is the observed and |F_c| the calculated structure factor amplitude.

^d Rfree is the same as R calculated with a randomly selected test set of 5% (HR3066a^a) or 5.3% (Au10pe) reflections that were never used in refinement calculations.