**Supplementary file 1. X-ray data collection and structural refinement statistics.**

|  |  |
| --- | --- |
| **Data collection** | |
| Space group | P1 |
| a, b, c (Å) | 39.06, 51.01, 76.56 |
| α, β, γ (°) | 103.49, 101.78, 96.07 |
| Resolution (Å) | 46.60-1.69 (1.72-1.69) |
| Rmerge | 0.06 (0.96) |
| Rmeas | 0.07 (1.13) |
| Rpim | 0.04 (0.59) |
| Mean I/σ (I) | 13.7 (1.8) |
| CC1/2 | 1.00 (0.69) |
| Total reflections | 428,508 (18,156) |
| Unique reflections | 60,345 (2,695) |
| Completeness (%) | 96.6 (84.6) |
| Multiplicity | 7.1 (6.7) |
| **Refinement** | |
| Rwork | 0.19 |
| Rfree | 0.23 |
| RMS bonds (Å) | 0.00 |
| RMS angles (°) | 0.85 |
| Ramachandran favored (%) | 98.68 |
| Ramachandran outliers (%) | 0 |
| Rotamer outliers (%) | 0.19 |
| Clashscore | 2.15 |
| Average B-factor of the protein (Å2) | 41.99 |
| Average B-factor of the ligand (Å2) | 34.14 |
| C-beta outliers | 0 |

1. The statistics are based on the calculations from Aimless and MolProbity.

2. The numbers in parentheses represent the highest resolution shell.

3. Rmerge = ∑hkl ∑j |Ihkl,j - < Ihkl > | / (∑hkl∑jIhkl,j); Rmeas = ∑hkl [N/(N-1)]1/2 ∑j |Ihkl,j - < Ihkl > | / (∑hkl∑jIhkl,j); Rpim = ∑hkl [1/(N-1)]1/2 ∑j |Ihkl,j - < Ihkl > | / (∑hkl∑jIhkl,j)

4. Rwork = ∑hkl |Fobshkl - Fcalchkl| / ∑|Fobshkl|; Rfree is equivalent to Rwork, with 5% of data excluded from refinement process. |Fobshkl| and |Fcalchkl| represent the observed and calculated structure factor amplitudes.