|  |  |
| --- | --- |
| **Condition** | **Parameter** |
| Diffraction source | MX 14.2, BESSY II |
| Wavelength (Å) | 0.9184 |
| Temperature (K) | 100 |
| Detector | PILATUS3S 2M |
| Crystal-detector distance (mm) | 251.228 |
| Rotation range per image (°) | 0.10 |
| Total rotation range (°) | 360 |
| Exposure time per image (s) | 0.05 |
| Space group | *R*32 (155) |
| Cell dimensions |
| a, b, c (Å) | 53.80, 53.80, 64.33 |
| Α, β, γ (°) | 90.00, 90.00, 120.00 |
| Resolution (Å) | 37.73-2.20 (2.26-2.20)  |
| Multiplicity | 19.22 (18.64) |
| Number of reflections |
| Total  | 36749 (5500) |
| Unique | 1912 (295) |
| Completeness (%) | 99.30 (98.00) |
| Rmaes\* (%) | 6.70 (61.10) |
| I/σ  | 28.83 (5.43) |
| Overall B factor from Wilson plot (Å2) | 48.73 |
| **Refinement statistics** |
| Resolution range (Å) | 37.73-2.20 (2.26-2.20) |
| No. of reflections, working set | 1816 (127) |
| Rwork† (%) / Rfree‡ (%) | 24.57/27.37 |
| Number of atoms |
| Protein | 297 |
| Water  | 13 |
| Ion | 2 (chloride) |
| Root mean square deviation |
| Bond lengths (Å) | 0.013 |
| Bond angles (°) | 1.650 |
| Average B factors (Å2) Overall | 57.29 |
| Ramachandran plot |
| Most favored region (%) | 97.30 (36/39)  |
| Allowed region (%)PDB code | 100 (39/39)7AL0 |

**Supplementary file 3.** Data collection and refinement statistics of X-ray diffraction. \*Rmeas is a redundancy-independent merging R factor. $R\_{meas}=\sum\_{hkl}^{}\left\{{N\left(hkl\right)}/{\left[N\left(hkl\right)-1\right]}\right\}^{{1}/{2}}\sum\_{i}^{}{\left|I\_{i}\left(hkl\right)-\left⟨I\left(hkl\right)\right⟩\right|}/{\sum\_{hkl}^{}\sum\_{i}^{}I\_{i}}\left(hkl\right)$, where $\left⟨I\left(hkl\right)\right⟩$ is the mean of the $N\left(hkl\right)$ individual measurements $I\_{i}\left(hkl\right)$ of the density of reflections$ hkl $†Rwork= ΣǀǀFoǀ - kǀ Fcǀǀ/Σ/FO ǀ, where Fo and Fc are the observed and calculated structure factors, respectively. ‡Rfree = defined by Brunger (***Brunger, 1992***).