**Table 1. Data collection and refinement statistics**

| **Data collection** | **Native** | **Derivative** |
|---|---|---|
| Wavelength, Å | 0.9123 | 1.5418 |
| Space group | $P6_422$ | $P6_422$ |
| Cell dimensions, Å | $a$ = 100.946 | $a$ = 101.002 |
| | $b$ = 100.946 | $b$ = 101.002 |
| | $c$ = 173.864 | $c$ = 174.483 |
| Resolution limits, Å | 61.66–1.65 | 30.92–1.83 |
| No. of reflections | 582,856 | 715,148 |
| No. of unique reflections | 58,965 | 46,388 |
| Completeness, % | 93.0 (66.9) | 98.5 (89.9) |
| Redundancy | 9.9 (6.2) | 15.4 (7.2) |
| $\langle I/\sigma(I)\rangle$ | 28.1 (5.8) | 24.4 (4.7) |
| $R_{merge}$ (%) | 0.055 (0.323) | 0.095 (0.338) |
| $R_{meas}$ (%) | 0.058 (0.353) | 0.098 (0.364) |
| **Refinement** | | |
| Resolution range, Å | 20.00–1.65 (1.69-1.65) | |
| Completeness (working + test), % | 92.76 (62.83) | |
| No. of reflections ($F > 0$) | 55,887 (2,737) | |
| Wilson B, $Å^2$ | 23.5 | |
| $R_{cryst}$, % | 15.58 (15.60) | |
| $R_{free}$, % | 17.83 (20.70) | |
| No. of non-hydrogen atoms | 3,725 | |
| Protein | 3,119 | |
| Water | 497 | |
| Sulfate | 40 | |
| Glycerol | 48 | |
| CL | 3 | |
| 1,3-butanediol | 30 | |
| TRIS | 8 | |
| rmsd from ideality | | |
| Bond lengths, Å | 0.014 | |

| Data collection | Native | Derivative |
|---|---|---|
| Bond angles, ° | 1.373 | |
| Dihedrals, ° | 17.3 | |
| Improper, ° | 0.33 | |
| **Average B-factor, Å$^2$** | 45.82 | |
| Protein atoms | 46.99 | |
| Main chain | 45.83 | |
| Water | 39.71 | |
| Glycerol | 40.52 | |
| $SO_4^{2-}$ | 41.42 | |
| CL | 68.70 | |
| 1,3-butanediol | 39.93 | |
| TRIS | 32.22 | |

$R_{merge} = \Sigma|I - \langle I \rangle| / \Sigma\langle I \rangle$.

Values in parentheses correspond to the highest resolution shell for data scaling (1.74–1.65 Å) and refinement ( 1.69-1.65 Å), respectively. For the derivative dataset, the highest resolution limit is 1.93 – 1.83 Å.

$R_{cryst} = \Sigma||F_{obs}| - |F_{calc}||/\Sigma|F_{obs}|$.

$R_{free}$ is calculated as for $R_{cryst}$ but for a test set comprising reflections not used in the refinement (5.1%).