|  |  |  |
| --- | --- | --- |
|  | Native | Peak |
| Wavelength [Å] | 0.97530Å | 0.97857 Å |
| Resolution [Å] | 57.07-2.7(2.83-2.7) \* | 56.82-2.9(3.1-2.9) \* |
| Space group | P 31 2 1 | P 31 2 1 |
| Cell parameters:  a,b,c [Å] α,β,γ [°] | 114.1, 114.1, 67.8490, 90, 120  | 113.65, 113.65, 67.6090, 90, 120  |
| Rmerge ‡ [%] | 17.8 (63.8) \* | 12.9 (72.5) \* |
| Rpim [%] | 8.6 (31.9) \* | 5.5 (30.8) \* |
| *I* / δ*I* | 7.5 (3.0) \* | 11.6 (2.4) \* |
| *CC(1/2)* [%] | 99.3 (84.8) \* | 99.8 (87.6) \* |
| Completeness [%] | 99.9 (100.0) \* | 100 (100) \* |
| Redundancy | 9.9 (9.5) \* | 12.3 (12.5) \* |
| **Refinement** |  |  |
| Resolution [Å] | 43.67-2.70 (2.8-2.7) \* |  |
| No. reflections | 14280 |  |
| *R*work / *R*free § [%]  | 22.11/28.26 |  |
| No. atoms |  |  |
|  Protein | 2258 |  |
|  Ligand | 6 |  |
|  Water | 54 |  |
| *B*-factors [Å2] |  |  |
|  Protein | 41.359 |  |
|  Ligand | 46.488 |  |
|  Water | 27.491 |  |
| Ramachandran Plot (%) |  |  |
|  Preferred region | 97.8 |  |
|  Allowed region | 2.2 |  |
|  Outliers | 0.0 |  |
| R.m.s deviations |  |  |
|  Bond lengths (Å) | 0.008 |  |
|  Bond angles (°) | 1.008 |  |
| PDB code | 5C9S |  |