表1-1 mNMNAT3数据收集以及结构精修的信息

Table 1.1Data collection and structure refinement statistics of mNMNAT3.

|  |  |
| --- | --- |
| Name | mNMNAT3 |
| **Data collection** |  |
| BeamLine/detector | SSRF BL17U/ ADSC Quantum 315r |
| Wavelength (Å) | 0.9791 |
| Space group | *P*21 |
| Cell dimensions (Å, º) | a = 53.7, b = 80.8, c = 64.5α= γ = 90，β = 102.2  |
| Resolution (Å)a | 2.00 (2.07-2.00) |
| No. of measured reflections | 192927 |
| No. of unique reflectionsa | 35818 (3645) |
| Redundancya | 5.4 (5.5) |
| Completeness (%)a | 98.2 (100) |
| Average (I/σ)a | 11.5 (5.2) |
| *R*merge (%)a,b | 0.102 (0.376) |
| **Refinement** |  |
| No. of reflections | 35772 |
| Rwork/Rfreec | 0.1985 / 0.2415 |
| No. of non-H atoms |  |
| Protein | 3531 |
| Waters | 119 |
| Ligand | 0 |
| Average B factor [A2] | 45.4 |
| RMS deviations |  |
| Bond lengths (Å) | 0.009 |
| Bond angles (°) | 1.089 |
| Ramachandran plot favored (%) | 95.08 |
| Ramachandran plot allowed (%) | 3.75 |
| Ramachandran plot outliers (%) | 1.17 |

aNumbers in parentheses are values for the highest-resolution shell.b*R*merge = ∑*hkl*∑i|*I*i -〈*I*〉|/∑*hkl*∑i|〈*I*〉|, where Ii is the intensity for the *i*th measurement of an equivalent reflection with indices h, k, and l.c*R*free was calculated with the 5% of reflections set aside randomly throughout the refinement.