

SUPPLEMENTARY DATA

Table S1. Data collection and refinement statistics

| | PNK-FHA | PNK-FHA / XRCC1 |
|---|--------------------------|------------------------|
| PDB accession code | 2BRF | 2W3O |
| Data collection | | |
| Space group | P2 ₁ | P3 |
| Cell dimensions | | |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 31.81, 40.05, 37.51 | 56.90, 56.90, 62.77 |
| α , β , γ (°) | 90, 90.96, 90 | 90, 90, 120 |
| Resolution (Å) | 37.50- 1.40 (1.44-1.40)* | 38.75-1.85 (1.95-1.85) |
| <i>R</i> _{merge} | 0.050 (0.16) | 0.069 (0.299) |
| Mn // σ I | 18.4 (6.3) | 13.3 (2.3) |
| Completeness (%) | 97.2 (88.0) | 99.0 (95.3) |
| Redundancy | 3.4 (2.4) | 3.4 (2.1) |
| Refinement | | |
| Resolution (Å) | 37.5 – 1.40 | 37.85-1.85 |
| No. unique reflections | 15643 | 19211 |
| <i>R</i> _{work} / <i>R</i> _{free} | 0.15 / 0.18 | 0.18 / 0.24 |
| No. atoms | | |
| Protein | 775 | 1508 |
| Peptide | | 148 |
| Ion | 10 | 6 |
| Water | 144 | 286 |
| B-factors | | |
| Protein | 9.5 | 25.7 |
| Peptide | n/a | 29.7 |
| Ion | 19.4 | 54.7 |
| Water | 9.5 | 36.9 |
| R.m.s deviations | | |
| Bond lengths (Å) | 0.009 | 0.018 |
| Bond angles (°) | 1.320 | 1.715 |

* Highest resolution shell is shown in parenthesis