**Figure 6 – source data 2.** **Crystallographic data collection and refinement statistics for Δloop-nDsbDox**

|  |  |
| --- | --- |
| **Unit Cell** | |
| Space Group | P21 |
| Cell dimensions (Å) | *a* = 37.33, *b* = 81.34, *c* = 46.39, β=100.66o |
| **Data Collection** | |
| Temperature (K) | 100 |
| Wavelength (Å) | 1.5418 |
| Resolution (Å) | 39.77 to 2.60 (2.74 to 2.60)\* |
| <I/σ> | 5.4 (3.3)\* |
| Rmeas | 0.31 (0.38)\* |
| Multiplicity | 3.1 (2.9)\* |
| **Refinement** | |
| Refinement program | Phenix.refine |
| Number of unique reflections used | 6808 |
| Completeness (%) | 80.7 (79.0)\* |
| R-factor (%) | 25.2 |
| Rfree (%) | 29.2 |
| Average B (Å2) | 26.0 |
| r.m.s.d. bond lengths (Å) | 0.003 |
| r.m.s.d. bond angles (°) | 0.721 |
| **Ramachandran** | |
| Favoured | 211 (95.0%) |
| Allowed | 9 (4.1%) |
| Outliers | 2 (0.9%) |
| **Asymmetric unit contents** | |
| Polypeptide chains | 2 |
| No. of atoms: total/non-solvent | 1838/1779 (13 in alternative conformations) |

\* values in parentheses are for corresponding highest resolution cell

Rsym = Σ |Ih – <Ih>|/ Σ Ih

R-factor = Σ (|Fobs| - |Fcalc|)/ Σ |Fobs|

r.m.s.d. = root mean square deviation