|  |  |
| --- | --- |
|  | **Stu2 CTS bound to dwarf Ndc80c\***  |
| **Wavelength**  | 0.97918 Å  |
| **Resolution range**  | 42.72 - 2.72 (2.817 - 2.72)  |
| **Space group**  | C 2 2 21  |
| **Unit cell** | 170.886 183.175 124.317 90 90 90  |
| **Total reflections**  | 697683 (62919)  |
| **Unique reflections**  | 52106 (4719)  |
| **Multiplicity**  | 13.4 (13.3)  |
| **Completeness (%)**  | 99.03 (91.15)  |
| **Mean I/sigma(I)**  | 18.40 (1.78)  |
| **Wilson B-factor**  | 63.68  |
| **R-merge**  | 0.1071 (0.9043)  |
| **R-meas** | 0.1114 (0.9395)  |
| **R-pim** | 0.03047 (0.2529)  |
| **CC1/2** | 0.999 (0.829)  |
| **CC\*** | 1 (0.952)  |
| **Reflections used in refinement**  | 52103 (4719)  |
| **Reflections used for R-free**  | 2013 (194)  |
| **R-work**  | 0.1976 (0.2789)  |
| **R-free** | 0.2416 (0.2910)  |
| **CC(work)** | 0.962 (0.822)  |
| **CC(free)** | 0.960 (0.757)  |
| **Number of non-hydrogen atoms**  | 5994  |
|  **macromolecules**  | 5869  |
|  **ligands** | 30  |
|  **solvent**  | 95  |

**Supplementary File 3. Data collection and refinement statistics.**

|  |  |
| --- | --- |
| **Protein residues**  | 713 |
| **RMS(bonds)** | 0.005  |
| **RMS(angles)**  | 0.74  |
| **Ramachandran favored (%)**  | 97.57  |
| **Ramachandran allowed (%)**  | 2.43  |
| **Ramachandran outliers (%)**  | 0.00  |
| **Rotamer outliers (%)**  | 0.15  |
| **Clashscore** | 6.46  |
| **Average B-factor**  | 88.87  |
|  **macromolecules**  | 89.23  |
|  **ligands**  | 89.23  |
|  **solvent** | 63.61 |
|  **Number of TLS groups**  | 1 |

Statistics for the highest-resolution shell are shown in parentheses.