

**Supplementary Table S1. X-ray data collection and refinement statistics for the native full-length HIV-1 CA / ZW-1261 complex (PDB ID: 7M9F).**

|                                    |                               |
|------------------------------------|-------------------------------|
| <b>Data collection</b>             | Beamline APS 22-ID            |
| Wavelength (Å)                     | 1.00000                       |
| Resolution (Å)                     | 2.70 (2.70-2.77) <sup>a</sup> |
| Space group                        | P6                            |
| Cell dimensions                    |                               |
| a, c (Å)                           | 90.9, 56.1                    |
| Observed reflections               | 52,178                        |
| Unique reflections                 | 7,239                         |
| Redundancy                         | 7.2 (6.1)                     |
| Completeness (%)                   | 97.9 (91.1)                   |
| R <sub>meas</sub> <sup>b</sup>     | 0.118 (0.84)                  |
| CC <sub>1/2</sub>                  | 99.6 (78.3)                   |
| Avg I/σ                            | 13.6 (3.4)                    |
| <b>Refinement statistics</b>       |                               |
| Resolution (Å)                     | 45.71-2.70                    |
| No. of reflections (working)       | 6,881                         |
| No. of reflections (test)          | 356                           |
| R <sub>work</sub> <sup>c</sup>     | 0.197                         |
| R <sub>free</sub> <sup>d</sup>     | 0.253                         |
| Overall B value (Å <sup>2</sup> )  | 70.0                          |
| Wilson B value (Å <sup>2</sup> )   | 63.5                          |
| Ramachandran plot (%) <sup>e</sup> |                               |
| Favored                            | 95%                           |
| Allowed                            | 4.5                           |
| Disallowed                         | 0.5                           |
| All-atom clashscore                | 4                             |
| RMSD Bond length (Å)               | 0.002                         |
| RMSD Angle (°)                     | 0.994                         |

<sup>a</sup> Values in parentheses are for the outer resolution shell.

$$^b R_{\text{meas}} = \frac{\sum_{hkl} \sqrt{\frac{n}{n-1}} \sum_{j=1}^n |I_{hkl,j} - \langle I_{hkl} \rangle|}{\sum_{hkl} \sum_j I_{hkl,j}}$$

$$^c R_{\text{cryst}} = \frac{\sum_{hkl} |F_{\text{obs}} - F_{\text{calc}}|}{\sum_{hkl} |F_{\text{obs}}|}$$

<sup>d</sup> R<sub>free</sub> = R<sub>cryst</sub>, except 5% of the data excluded from the refinement.

<sup>e</sup> Evaluated by MolProbity (Chen *et al.*, *Acta Cryst.* D66, 2010, 12-21).