|  |  |
| --- | --- |
| Data Collection for CPXV203/OVA:H-2Kb:h2ma |  |
| Space Group | P 1 |
| Cell dimensions |  |
| a, b, c (Å) | 88.31, 88.25, 106.42 |
| , ,  (o) | 76.18, 69.29, 66.69 |
| Data Set | SeMet |
| Wavelength (Å) | 0.97909 |
| X-ray Source | ALS 4.2.2b |
| Resolution (Å) overall (outer shell) | 50-3.0 (3.19-3.00) |
| Observations/Unique | 198533/47950 |
| Multiplicity | 4.1 (4.2) |
| Completeness (%) | 87.9 (84.9) |
| R-sym (%) | 16.4 (62.2) |
| I/ | 7.3 (2.6) |
| Refinement Statisticsc |  |
| Complexes in ASU | 4 |
| Reflections Rwork/Rfree | 47881/2394 |
| #Residues/Protein Atoms/Solvent | 2284/18596/72 |
| Rwork overall (outer shell) (%) | 22.9 (31.6) |
| Rfree overall (outer shell) (%) | 25.3 (35.5) |
| RMSD bond lengths (Å)/angles (o) | 0.002/0.538 |
| RMSD Dihedral (o) | 9.662 |
| Ramachandran plotd |  |
| Favored/Allowed/Outliers (%) | 97.2/2.8/0.0 |
| Estimated Coordinate Error (Å) | 0.46 |
| Structural Analysis |  |
| Clashscored | 8.56 |
| Bound vs. free MHCI C RMSD (Å)e |  |
| (HC, 1/2, 3, 2m\*, OVA) | 1.61, 0.42, 0.71, 0.45\*, 0.28 |

**Table S2. Summary of Data Collection, Phasing, and Refinement.**

aValues as defined in HKL2000 [53].

bAdvanced Light Source, Beamline 4.2.2

cValues as defined in PHENIX [56].

dMolProbity scores output within PHENIX.

eReference PDBs: 1VAC (H-2Kb:m2m), \*2F74 (H-2Db:h2m).