**Table S4. CPXV203/MHCI interactions.**

**Hydrogen bondsa**

|  |  |  |  |
| --- | --- | --- | --- |
| **Structural Elementb** | **CPXV203** | **H-2Kb 2 domain** | **Length (Å)** |
| h4 | L157 O | E128 N | 3.1 |
| looph4-h5 | S159 O | E128 O2 | 2.3 |
|  | S159 N | E128 O2 | 3.4 |
|  | Y161 OH | Q114 N | 3.3 |
|  | Y161 OH | L126 O | 2.6 |
|  | E162 O1 | R111 N1 | 4.9 (LRE)c |
|  | E162 O2 | R111 N1 | 3.5 (LRE)c |
|  |  | **H-2Kb 3 domain** |  |
| loopb1-b2 | R31 N1 | D227 O1 | 2.9 |
|  | R31 N2 | D227 O1 | 2.9 |
| loopb5-b6 | G77 N | Q226 O | 2.7 |
|  | V78 N | E229 O1 | 2.6 |
|  | T79 O1 | E229 O2 | 2.4 |
|  | T79 N | E229 O1 | 3.3 |
| b6 | H80 N2d | E229 O2 | 3.5 |
|  |  | **2m** |  |
| b8 | H119 N2 | T86 O | 3.0 |
|  | Y123 O | Q2 N | 3.2 |
|  | E125 N | M0 Oe | 2.8 |
|  | E125 O | M0 Ne | 2.4 |
| b10 | N141 O1 | K91 N | 3.1 |
|  | H142 N2 | T4 O | 2.7 |
| looph4-h5 | E162 O1 | K58 N | 2.9 |
|  | T165 O1 | D59 O2 | 2.9 |

**Contacts <4.0 Åa,f**

|  |  |  |
| --- | --- | --- |
| **Structural Elementb** | **CPXV203** | **H-2Kb 2 domain** |
| h4 | E154 (2) | T134 |
| looph4-h5 | I160 (2) | E128 |
|  | Y161 (5) | Y113, Q115 (3), A125 |
|  |  | **H-2Kb 3 domain** |
| loopb1-b2 | R31 (1) | Q226 |
| b5 | F76 (3) | Q226 |
| loopb5-b6 | G77 (2) | M228, E229 |
| looph4-h5 | K171 (1) | T214 |
| h5 | T175 (1) | I225 |
|  | Y179 (6) | I225 (2), Q226 (4) |
|  |  | **2m** |
| b8 | L121 (2) | T4, T86 |
| b10 | H142 (2) | K6 |

aContacts calculated with HBPLUS.

bStructural element refers to CPXV203.

c(LRE) = Long range electrostatics (3.5-5.0 Å) calculated with NCONT.

dIdentified by model inspection.

eArtifact contacts due to use of refolded h2m.

fNumber of non-bonded contacts listed in parentheses.