**Supplementary file 4. Electrostatic Interactions between B1E11K Fabs and RESA P2 (16AA) peptide.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **RESA P2** | **Fab A Heavy** | **Fab A Kappa** | **Fab B Heavy** | **Fab B Kappa** |
| **E1\*** |  | **H49\*** |  |  |
| **E2\*** | **R94\*** |  |  |  |
| **E2 [O]** | **S96 [N]** |  |  |  |
| **E2 [O]** | **G97 [N]** |  |  |  |
| **N3 [Nd2]** | **S31 [O]** |  |  |  |
| **N3 [Od1]** | **W33 [N]** |  |  |  |
| **V4 [N]** | **S96 [Og]** |  |  |  |
| **V4 [O]** | **S96 [Og]** |  |  |  |
| **V4 [O]** |  | **R96 [Nh]**  |  |  |
| **E5 [O]** |  | **R96 [Nh]** |  |  |
| **E5 [Oe]** |  |  |  | **G57 [N]** |
| **E6\*** |  | **R96\*** |  |  |
| **E6 [Oe]** |  | **S94 [N]** |  |  |
| **E6 [O]** |  |  |  | **H49 [Ne2]** |
| **N7 [N]** |  | **G92 [O]** |  |  |
| **N7 [Nd2]** |  | **G92 [O]** |  |  |
| **E9\*** |  | **R93\*** |  |  |
| **E10\*** |  |  | **R94\*** |  |
| **E10 [O]** |  |  | **S96 [N]** |  |
| **E10 [O]** |  |  | **G97 [N]** |  |
| **N11 [Nd2]** |  |  | **S31 [O]** |  |
| **N11[Od1]** |  |  | **W33 [N]** |  |
| **V12 [N]** |  |  | **S96 [Og]** |  |
| **V12 [O]** |  |  | **S96 [Og]** |  |
| **V12 [O]** |  |  |  | **R96 [Nh]** |
| **E13\*** |  |  | **R52\*** |  |
| **E13 [Oe]** |  |  | **W33 [Ne1]** |  |
| **E14\*** |  |  |  | **R96\*** |
| **E14 [Oe]** |  |  |  | **S94 [N]** |
| **E14 [Oe]** |  |  |  | **S94 [Og]** |
| **N15 [N]** |  |  |  | **G92 [O]** |
| **N15 [Nd2]** |  |  |  | **G92 [O]** |

The asterisk (\*) denotes a salt bridge. Atoms involved in hydrogen bonding interactions are shown in square brackets.