**Supplementary File 3**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Antigen (BSA Å2)** | **Interaction** | **3D11-HC** | **3D11-KC** |
|  |  | **Pro25 (7)** | vdW |  | Ser56 |
|  |  | **Pro27 (12)** | vdW | Tyr32 |  |
|  |  | **Pro28 (99)** | vdW | Tyr32, Ala95, Ala101 |  |
|  |  | ProO | HB | Tyr32OH |  |
|  |  | **Asn29 (105)** | vdW |  | Tyr32, Arg46, Ser49, Leu50, Glu53 |
|  |  | AsnND2 | HB |  | Glu53OE1 |
|  |  | AsnO | HB |  | Arg46NH1 |
|  |  | **Pro30 (71)** | vdW | Ala95 | Arg46 |
|  |  | **Asn31 (153)** | vdW |  | Asn34, Arg46, Trp89 |
|  |  |  | SB |  |  |
|  |  | AsnND2 | HB | Ala95O |  |
|  |  | AsnO |  |  | Asn34ND2 |
|  |  | **Asp32 (98)** | vdW | Asn33, His35 | Asn34, Gly91, Arg96 |
|  |  | AspO | HB | Asn33ND2 |  |
|  |  | AspOD1 | HB,SB | Asn33ND2 | Arg96NH2, Arg96NE |
|  |  | AspOD2 | HB,SB | His35NE2 |  |
|  |  | **Pro33 (103)** | vdW |  | Tyr27D, Tyr32, Gly91 |
|  |  | ProO | HB | Asn33ND2 |  |
|  |  | **Pro34 (41)** | vdW | Tyr52, Asn33 |  |
|  |  | **Pro35 (106)** | vdW | Tyr50, Tyr52, Asn58 |  |
|  |  | **Pro36 (13)** | vdW | Asn54, Lys56 |  |
|  |  | ProO | HB | Asn54ND2 |  |
|  |  | **Asn37 (13)** | vdW | Asn54 |  |
|  |  | AsnOD1 | HB | Asn54ND2 |  |
|  |  | **Ala38 (2)** | vdW | Asn54 |  |
| **H-bonds** |  | 13 |  |  |  |
| **Salt Bridges** |  | 4 |  |  |  |
| **Core epitope\* BSA (Å2)** |  | 776 |  |  |  |
| **Total BSA (Å2)** |  | 823 |  |  |  |
|  |  |  |  |  |  |

\*Core epitope consists of residues 28 to 35 in PbCSP (PNPNDPPP)

vdW: van der Waals interaction (5.0 Å cut-off)

HB: hydrogen bond (3.8 Å cut-off)

SB: salt bridge (4.0 Å cut-off)