**S1 Table. Root mean square deviations (rmsd) between deposited and re-refined structures of 20 amino acid residues in the active site of DPP-4 complexes. All values are in Å.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  |  |  |  |
| Residues  | Sitagliptin **1** | Linagliptin **2** | Alogliptin **3** | Teneligliptin **4** |
|  |  |  |  |  |
| Trp629 | 0.05  | 0.07  | 0.04  | 0.02  |
| His740 | 0.02  | 0.06  | 0.06  | 0.05  |
| Ser630 | 0.10  | 0.03  | 0.04  | 0.02  |
| Tyr547 | 0.08  | 0.10  | 0.07  | 0.03  |
| Tyr631 | 0.03  | 0.14  | 0.05  | 0.04  |
| Phe357 | 0.06  | 0.12  | 0.03  | 0.03  |
| Pro550 | 0.20  | 0.09  | 0.22  | 0.02  |
| Tyr666 | 0.05  | 0.07  | 0.03  | 0.03  |
| Val656 | 0.08  | 0.04  | 0.02  | 0.04  |
| Trp659 | 0.07  | 0.06  | 0.04  | 0.03  |
| Tyr662 | 0.05  | 0.05  | 0.03  | 0.05  |
| Val711 | 0.06  | 0.04  | 0.04  | 0.03  |
| Asn710 | 0.06  | 1.11  | 0.06  | 0.04  |
| Arg125 | 0.29  | 0.14  | 0.10  | 0.13  |
| Arg669 | 0.05  | 1.01  | 0.05  | 0.05  |
| Glu205 | 0.07  | 0.10  | 1.03  | 0.03  |
| Glu206 | 0.06  | 0.09  | 0.03  | 0.08  |
| Arg358 | 0.13  | 0.81  | 0.08  | 0.08  |
| Ser209 | 0.05  | 0.09  | 0.04  | 0.04  |
| Val207 | 0.05  | 0.07  | 0.03  | 0.03  |
|  |  |  |  |  |