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| --- | --- | --- | --- |
| **Vaccine** | **TLR4** | **MHC1** | **MHC2** |
| HADDOCK Score | -31.1 +/- 17.3 | -20.4 +/- 5.9 | -75.9 +/- 12.6 |
| Cluster size | 8 | 4 | 5 |
| RMSD | 1.6 +/- 1.3 | 9.4 +/- 0.2 | 18.0 +/- 0.1 |
| Van der Waals energy | -89.0 +/- 12.4 | -91.4 +/- 12.3 | -86.5 +/- 10.4 |
| Electrostatic energy | -531.3 +/- 44.1 | -286.9 +/- 54.2 | -699.9 +/- 61.5 |
| Desolvation energy | 17.5 +/- 6.9 | 3.4 +/- 1.4 | 19.8 +/- 1.9 |
| Restraints violation energy | 9754.4 +/- 400.8 | 2753.7 +/- 315.7 | 2620.8 +/- 208.7 |
| Buried Surface Area | 2544.7 +/- 134.1 | 3563.8 +/- 289.6 | 3966.6 +/- 209.0 |
| Z-Score | -2.0 | -1.6 | -1.7 |