**S1 Table. Three-dimensional structures of VS0-4.** Five possible conformations were predicted by homology-based modeling and refined by molecular dynamics.

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| --- | --- | --- |
| Conformation  | Number of structures | Existence time (ns) |
| 1 | v04_5.png | 52 | 1.04 |
| 2 | v04_2.png | 759 | 15.18 |
| 3 | v04_1.png | 1348 | 26.96 |
| 4 | v04_4.png | 290 | 5.8 |
| 5 | v04_3.png | 51 | 1.02 |