Table S1 Statistical analysis results of RMSD, Rg and SASA for HvLD at different temperatures

|  |  |  |
| --- | --- | --- |
| 　 | 318 K / 298 K | 343 K / 298 K |
| 　 | SS | F | P-value | SS | F | P-value |
| RMSD | 2.53  | 169.29  | 1.5093E-38 | 159.38 | 6487.75  | 0 |
| Rg | 1.01  | 134.13  | 6.4376E-31 | 147.65  | 15301.80  | 0 |
| SASA | 8.09E+07 | 474.79  | 4.70E-104 | 1.01E+08 | 616.26  | 5E-134 |
|  | 318 K / 298 K (system without Ca2+) | 343 K / 298 K (system without Ca2+) |
|  | SS | F | P-value | SS | F | P-value |
| RMSD | 1021.63  | 11205.34  | 0 | 6294.85  | 7388.65  | 0 |
| Rg | 73.84  | 2066.27  | 0 | 988.23  | 10377.55  | 0 |
| SASA | 3.50E+09 | 10770.46  | 0 | 3.03E+08 | 682.94  | 5E-148 |

Table S2 Length and occupancy of important hydrogen bond interactions of HvLD at 298K, 318K, and 343K.

|  |  |  |  |
| --- | --- | --- | --- |
| Hydrogen Bond | 298 K | 318 K | 343 K |
| Occupancy (%) | Distance (Å) | Angle (˚) | Occupancy (%) | Distance (Å) | Angle (˚) | Occupancy (%) | Distance (Å) | Angle (˚) |
| ASP815@OD1 | ASN817@N | 99.64  | 2.90  | 160.53  | 59.00  | 2.91  | 159.39  | 55.80  | 2.93  | 158.48  |
| ASN403@OD1 | HIS404@ND1 | 99.92  | 2.77  | 155.77  | 98.14  | 2.78  | 156.26  | 60.10  | 2.78  | 158.18  |
| GLU435@O | ASN442@N | 99.80  | 2.94  | 161.04  | 99.58  | 2.99  | 160.21  | 66.91  | 3.02  | 160.56  |
| ASN442@OD1 | ALA438@N | 99.73  | 3.00  | 160.67  | 99.73  | 2.98  | 159.82  | 58.25  | 2.99  | 157.95  |
| GLU381@OE2 | SER371@OG | 99.73  | 2.63  | 163.51  | 54.29  | 2.76  | 159.59  | 53.52  | 2.74  | 160.23  |
| ARG542@O | GLN590@NE2 | 99.69  | 2.89  | 161.43  | 98.48  | 2.90  | 162.03  | 85.52  | 2.90  | 160.48  |
| GLU516@OE2 | ASN442@ND2 | 99.57  | 2.85  | 160.49  | 99.93  | 2.83  | 161.84  | 58.33  | 2.84  | 159.19  |
| SER677@OG | ASN636@ND2 | 99.28  | 2.94  | 159.36  | 98.34  | 2.95  | 154.67  | 86.32  | 3.00  | 155.46  |
| THR580@O | LEU584@N | 99.20  | 2.97  | 161.67  | 91.60  | 3.04  | 159.93  | 87.06  | 3.07  | 160.50  |
| SER135@O | ARG182@NH1 | 99.17  | 2.84  | 155.81  | 98.44  | 2.85  | 155.61  | 85.04  | 2.86  | 154.52  |
| VAL175@O | SER172@N | 99.12  | 2.94  | 157.52  | 98.40  | 2.96  | 156.99  | 83.38  | 2.96  | 156.13  |
| GLU381@OE1 | SER371@N | 99.08  | 2.83  | 152.28  | 81.14  | 2.97  | 149.06  | 50.14  | 2.96  | 148.46  |
| ASP338@O | GLN341@NE2 | 98.99  | 2.92  | 158.44  | 97.47  | 2.92  | 158.44  | 75.88  | 2.94  | 158.67  |
| ASN436@OD1 | ASN441@N | 98.75  | 2.96  | 161.38  | 97.25  | 2.98  | 160.82  | 57.25  | 2.96  | 157.94  |
| VAL798@O | HIS786@N | 98.74  | 2.96  | 160.68  | 97.99  | 2.98  | 160.64  | 73.82  | 3.09  | 156.43  |
| ILE261@O | SER265@OG | 98.59  | 2.69  | 163.25  | 92.60  | 2.79  | 157.84  | 86.00  | 2.81  | 155.99  |
| SER172@O | VAL175@N | 98.45  | 3.01  | 153.17  | 96.97  | 3.02  | 152.93  | 81.29  | 3.04  | 153.04  |
| ILE764@O | SER767@OG | 98.37  | 2.68  | 165.21  | 95.99  | 2.70  | 164.89  | 83.67  | 3.09  | 146.40  |
| GLU568@O | GLN559@NE2 | 98.28  | 2.97  | 156.83  | 95.22  | 2.95  | 158.85  | 84.78  | 2.95  | 156.77  |
| GLY375@O | SER215@OG | 98.05  | 2.75  | 155.90  | 82.78  | 2.79  | 153.48  | 77.10  | 2.80  | 151.70  |
| SER437@OG | ASN442@ND2 | 97.88  | 2.91  | 144.07  | 97.67  | 2.93  | 142.22  | 56.76  | 2.91  | 144.45  |
| PRO334@O | SER337@N | 97.47  | 3.07  | 155.51  | 89.86  | 3.12  | 154.30  | 81.04  | 3.15  | 152.90  |
| SER177@O | LYS170@N | 97.34  | 3.03  | 161.69  | 95.85  | 3.04  | 161.33  | 84.07  | 3.03  | 160.41  |
| ILE347@O | GLU350@N | 97.21  | 2.97  | 150.56  | 96.74  | 3.01  | 153.41  | 57.70  | 3.05  | 151.63  |
| SER767@OG | HIS847@NE2 | 96.79  | 2.91  | 148.12  | 92.92  | 2.94  | 147.11  | 86.98  | 2.98  | 147.53  |
| PRO624@O | ARG542@NE | 95.94  | 3.00  | 145.57  | 93.58  | 3.05  | 142.67  | 72.97  | 3.01  | 145.36  |
| GLN341@OE1 | SER725@N | 95.88  | 3.04  | 161.43  | 93.57  | 3.03  | 162.79  | 77.81  | 3.04  | 160.08  |
| ASP648@O | VAL652@N | 95.78  | 2.94  | 146.47  | 81.48  | 3.03  | 142.31  | 77.18  | 3.07  | 145.86  |
| GLY409@O | SER415@OG | 95.70  | 2.77  | 160.97  | 89.03  | 2.79  | 162.50  | 62.95  | 2.78  | 161.71  |
| HIS292@O | LEU296@N | 95.51  | 3.08  | 156.09  | 87.77  | 3.12  | 155.52  | 76.51  | 3.18  | 154.86  |
| THR586@O | GLN590@N | 95.42  | 3.09  | 158.15  | 82.83  | 3.17  | 157.25  | 78.41  | 3.17  | 158.96  |
| GLY356@O | ASN358@N | 94.62  | 2.90  | 146.37  | 90.84  | 2.91  | 146.48  | 72.20  | 2.97  | 139.30  |
| ASP760@OD2 | SER853@OG | 94.27  | 2.67  | 164.69  | 93.47  | 2.67  | 164.73  | 60.19  | 2.65  | 164.47  |
| ASN525@O | ASN530@ND2 | 94.21  | 2.93  | 158.26  | 85.46  | 2.94  | 156.72  | 70.85  | 2.95  | 158.36  |
| MET674@O | SER677@N | 94.17  | 3.15  | 154.48  | 82.30  | 3.20  | 153.22  | 79.44  | 2.79  | 158.89  |
| ASN576@O | THR580@OG1 | 91.45  | 2.78  | 161.05  | 85.58  | 2.81  | 160.77  | 65.67  | 2.88  | 160.03  |
| VAL344@O | ILE347@N | 91.39  | 3.06  | 152.98  | 81.95  | 3.04  | 152.21  | 66.14  | 3.12  | 152.97  |
| PRO631@O | THR634@N | 89.15  | 3.16  | 154.64  | 84.77  | 3.17  | 155.36  | 71.77  | 3.19  | 155.88  |
| GLY22@O | ALA26@N | 89.06  | 3.02  | 145.49  | 79.64  | 2.98  | 143.55  | 70.58  | 3.03  | 147.04  |
| TRP461@O | VAL467@N | 87.95  | 3.17  | 163.54  | 74.10  | 3.21  | 163.28  | 64.58  | 3.22  | 162.51  |
| ASP648@OD2 | SER692@OG | 87.91  | 2.60  | 164.97  | 74.05  | 2.80  | 152.76  | 68.23  | 2.81  | 152.39  |
| LEU120@O | PHE124@N | 87.56  | 3.07  | 140.16  | 78.69  | 3.11  | 139.41  | 67.77  | 3.13  | 138.46  |
| GLN340@O | VAL344@N | 85.08  | 3.16  | 154.75  | 63.27  | 3.19  | 154.74  | 55.77  | 3.19  | 153.50  |
| MET339@O | ALA343@N | 84.69  | 3.12  | 151.41  | 73.38  | 3.12  | 150.89  | 68.99  | 3.12  | 150.17  |
| ASP110@OD1 | VAL111@N | 84.21  | 2.88  | 135.37  | 78.35  | 2.87  | 135.78  | 65.01  | 2.87  | 135.84  |
| LYS295@O | ALA299@N | 84.06  | 3.10  | 144.60  | 71.64  | 3.15  | 143.60  | 66.44  | 3.16  | 144.11  |
| GLN590@O | GLY594@N | 82.82  | 3.14  | 155.00  | 79.68  | 3.18  | 155.67  | 56.01  | 3.21  | 148.13  |
| LEU216@O | GLY375@N | 78.95  | 3.10  | 152.24  | 61.00  | 3.13  | 152.66  | 55.24  | 3.12  | 149.77  |
| LEU405@O | ASN441@ND2 | 78.21  | 3.08  | 161.17  | 77.33  | 3.05  | 160.91  | 56.32  | 3.07  | 156.86  |
| LEU241@O | GLU244@N | 78.00  | 2.99  | 140.63  | 67.10  | 3.02  | 138.79  | 64.03  | 3.01  | 140.04  |
| TRP705@O | ASN717@ND2 | 76.45  | 2.98  | 159.69  | 67.78  | 2.96  | 159.39  | 56.92  | 3.02  | 159.62  |
| GLU231@O | LYS234@N | 70.36  | 3.21  | 153.95  | 68.61  | 3.19  | 154.28  | 56.52  | 3.21  | 153.70  |
| ASP457@O | ASN460@ND2 | 70.31  | 3.15  | 153.96  | 59.44  | 3.14  | 156.34  | 58.91  | 3.12  | 155.28  |
| ASN441@OD1 | SER408@OG | 69.89  | 2.78  | 158.96  | 58.30  | 2.82  | 156.76  | 51.07  | 2.78  | 159.05  |
| ASP815@OD2 | SER768@OG | 69.65  | 2.91  | 136.65  | 58.57  | 2.64  | 165.63  | 54.11  | 2.65  | 165.13  |
| ASP710@OD2 | THR712@OG1 | 66.96  | 2.87  | 154.91  | 53.49  | 2.99  | 151.86  | 50.12  | 3.01  | 153.45  |