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| **Supplementary Data 1** | MD code for WT |
| **Supplementary Data 2** | Initial structure molecular dynamics of WT |
| Supplementary Data 3 | Molecular dynamics snapshot of WT at 1 microsecond |
| **Supplementary Data 4** | Molecular dynamics snapshot of WT at 1.5 microsecond |
| **Supplementary Data 5** | Molecular dynamics snapshot of WT at 4 microsecond |
| **Supplementary Data 6** | MD code for Y189A |
| **Supplementary Data 7** | Initial structure molecular dynamics of Y189A |
| Supplementary Data 8 | Molecular dynamics snapshot of Y189A at 1 microsecond |