|  |  |  |  |
| --- | --- | --- | --- |
| **Torsion Angle** | **Crystal Structure** | **Molecular Dynamics** | **Within Hypothesized Helix** |
|  | -40.1° | -38.7° | 57.9° |
|  | -6.8° | -9.2° | 2.1° |
|  | -60.1° | -46.9° | 57.2° |
| **RMSD (MD vs. crystal):** 0.23 Å | | | |