|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Model** | **GDT-HA** | **RMSD** | **MolProbity** | **Clash score** | **Poor rotamers** | **Rama favored** |
| Initial | 1.0000 | 0.000 | 2.224 | 15.9 | 1.5 | 94.2 |
| MODEL 1 | 0.9987 | 0.179 | 2.078 | 15.1 | 0.4 | 94.2 |
| MODEL 2 | 0.9993 | 0.180 | 2.106 | 16.2 | 0.7 | 94.2 |
| MODEL 3 | 0.9967 | 0.208 | 2.123 | 16.4 | 0.4 | 93.9 |
| MODEL 4 | 1.0000 | 0.183 | 2.136 | 17.5 | 0.7 | 94.2 |
| MODEL 5 | 0.9967 | 0.203 | 2.119 | 16.8 | 0.7 | 94.2 |

**VC1**

**VC2**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Model** | **GDT-HA** | **RMSD** | **MolProbity** | **Clash score** | **Poor rotamers** | **Rama favored** |
| Initial | 1.0000 | 0.000 | 2.294 | 16.1 | 1.5 | 93.1 |
| MODEL 1 | 0.9962 | 0.216 | 2.107 | 15.8 | 0.6 | 93.9 |
| MODEL 2 | 0.9973 | 0.186 | 2.109 | 14.8 | 0.9 | 93.3 |
| MODEL 3 | 0.9941 | 0.222 | 2.147 | 17.0 | 0.9 | 93.7 |
| MODEL 4 | 0.9968 | 0.189 | 2.159 | 16.7 | 0.9 | 93.3 |
| MODEL 5 | 0.9962 | 0.210 | 2.174 | 17.8 | 0.9 | 93.5 |