**Vina docking scores for the β3(+)–α1(-) intersubunit site**

|  |  |  |
| --- | --- | --- |
|  | Model Vina score | 6I53 Vina score |
| 3α5αP | -8.0 | -8.9 |
| 3β5αP | -7.9 | -8.7 |

**Vina docking scores for the α1 intrasubunit site**

|  |  |  |
| --- | --- | --- |
|  | Model Vina score | 6I53 Vina score |
| 3α5αP | -7.2 | -6.5 |
| 3β5αP | -7.4 | -6.1 |

**Vina docking scores for the β3 intrasubunit site**

|  |  |  |
| --- | --- | --- |
|  | Model Vina score | 6I53 Vina score |
| 3α5αP | -5.7 | -5.2 |
| 3β5αP | -5.5 | -4.6 |