**PIC Table 1**:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Types of inter-molecular interactions | | | | |
| S. No | Complex | Hydrogen bonds | Hydrophobic interactions | Aromatic-aromatic interactions | Cation-π interactions | Total number |
| 1 | G446V-DS9 | 5 | 12 | 0 | 2 | 19 |
| 2 | L452R-DS9 | 38 | 14 | 4 | 3 | 39 |
| 3 | Y453F-DS9 | 39 | 22 | 3 | 3 | 58 |
| 4 | S477G-DS9 | 25 | 14 | 5 | 2 | 29 |
| 5 | S477N-DS9 | 23 | 15 | 5 | 4 | 30 |
| 6 | S477R-DS9 | 8 | 20 | 1 | 2 | 26 |
| 7 | E484K-DS9 | 40 | 10 | 4 | 4 | 35 |
| 8 | E484A-DS9 | 23 | 16 | 4 | 3 | 43 |
| 9 | E484D-DS9 | 5 | 14 | 2 | 2 | 23 |
| 10 | E484G-DS9 | 17 | 15 | 2 | 0 | 24 |
| 11 | F490S-DS9 | 23 | 18 | 6 | 2 | 44 |
| 12 | N501Y-DS9 | 14 | 15 | 4 | 1 | 26 |