

|  | Energy of the complex | Energy of the binding pocket residues | Energy of the ligand | Nonbonding interaction energy |
|--|-----------------------|---------------------------------------|----------------------|-------------------------------|
| <b>AEA binding pose 1_H7_HC</b>                |                       |                                       |                      |                               |
| Equilibrated <i>pose1</i> (+1) <sup>a)</sup>   | -1757.21              | -1658.84                              | -69.02               | -29.35                        |
| Equilibrated <i>pose3</i> (+1) <sup>a)</sup>   | -1624.84              | -1522.59                              | -68.27               | -33.98                        |
| Equilibrated <i>pose8</i> (0) <sup>a)</sup>    | -2103.49              | -2005.02                              | -69.20               | -29.27                        |
| <b>AEA binding pose 1_H2/H3_HC</b>             |                       |                                       |                      |                               |
| Equilibrated <i>pose2</i> (0) <sup>a)</sup>    | -2684.86              | -2581.97                              | -66.14               | -36.75                        |
| Equilibrated <i>pose2'</i> (0) <sup>a)</sup>   | 2141.77               | -2039.22                              | -66.16               | -36.39                        |
| <b>AEA binding pose 2_HC<sub>a</sub>_H2/H3</b> |                       |                                       |                      |                               |
| Equilibrated <i>pose4</i> (+1) <sup>a)</sup>   | -1594.56              | -1500.03                              | -69.91               | -24.62                        |
| Equilibrated <i>pose5</i> (0) <sup>a)</sup>    | -2010.28              | -1912.38                              | -69.06               | -28.84                        |
| Equilibrated <i>pose6</i> (+1) <sup>a)</sup>   | -1797.92              | -1705.93                              | -66.90               | -25.09                        |
| Equilibrated <i>pose7</i> (+1) <sup>a)</sup>   | -1756.56              | -1658.92                              | -69.24               | -28.40                        |

<sup>a)</sup>The value in the parenthesis shows the total charge of the system.