|  |  |  |  |
| --- | --- | --- | --- |
|  | Affinity(kcal/mol) | H-bond | Picture |
| RK1 | -8.118 | GLU-180, THR-57, LYS-187 |  |
| RK2 | -9.617 | LYS-198, LYS-187, GLU-180, VAL-205 |  |
| Allapinin | -8.819 | GLU-180, THR-57 |  |
| Amiadaron | -8.33 | ASP-197 |  |

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**RK1**

mode | affinity | dist from best mode

| (kcal/mol) | rmsd l.b.| rmsd u.b.

-----+------------+----------+----------

1 -8.118 0 0

2 -7.885 1.324 2.132

3 -7.877 6.283 9.023

4 -7.829 4.705 9.015

5 -7.814 6.788 9.936

6 -7.778 3.786 11.52

7 -7.749 6.816 14.27

8 -7.725 6.275 11.6

9 -7.72 3.504 4.612

10 -7.7 3.082 4.734

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**RK2**

mode | affinity | dist from best mode

| (kcal/mol) | rmsd l.b.| rmsd u.b.

-----+------------+----------+----------

1 -9.617 0 0

2 -9.565 2.135 10.35

3 -9.56 0.4847 1.426

4 -8.981 1.788 2.56

5 -8.719 2.839 5.164

6 -8.667 15.62 20.06

7 -8.467 2.88 9.85

8 -8.218 16.12 20.52

9 -8.092 2.278 3.499

10 -8 2.244 10.66

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**Allapinin**

mode | affinity | dist from best mode

| (kcal/mol) | rmsd l.b.| rmsd u.b.

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1 -8.819 0 0

2 -8.588 1.226 2.322

3 -7.981 3.316 8.162

4 -7.969 3.717 8.503

5 -7.919 2.998 8.447

6 -7.7 2.87 8.167

7 -7.673 3.423 8.237

8 -7.574 30.42 31.99

9 -7.524 3.769 8.996

10 -7.359 3.045 5.672

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**Amiadaron**

mode | affinity | dist from best mode

| (kcal/mol) | rmsd l.b.| rmsd u.b.

-----+------------+----------+----------

1 -8.33 0 0

2 -7.905 3.887 7.415

3 -7.74 4.45 7.207

4 -7.693 2.577 10.13

5 -7.683 2.854 10.32

6 -7.621 2.333 5.3

7 -7.605 3.417 10.35

8 -7.578 3.852 8.888

9 -7.558 3.447 9.051

10 -7.392 3.146 5.947