| PDB   | AutodockVina | iDock | rdock-dock | rdock-dock_solv |
|-------|--------------|-------|------------|-----------------|
| 1AJU  | 3.2          | 2.6   | 1.2        | 1.2             |
| 1AM0  | 3.8          | 3.5   | 1.2        | 1.2             |
| 1BYJ  | 4.6          | 4.2   | 1.2        | 0.9             |
| 1EHT  | 3.5          | 1.9   | 0.5        | 0.5             |
| 1E12  | 5.3          | 5.4   | 4.5        | 4.6             |
| 1FMN  | 2.4          | 2.2   | 1.5        | 1.3             |
| 1FYP  | 5.0          | 5.3   | 1.1        | 1.2             |
| 1J7T  | 13.3         | 10.8  | 5.1        | 3.8             |
| 1KOC  | 3.1          | 3.0   | 1.2        | 1.4             |
| 1KOD  | 2.3          | 2.1   | 1.5        | 1.9             |
| 1MWL  | 11.3         | 11.5  | 4.8        | 5.0             |
| 1NBK  | 4.6          | 4.0   | 1.8        | 1.4             |
| 1NEM  | 5.6          | 5.6   | 2.3        | 1.9             |
| 1PBR  | 5.1          | 4.8   | 3.1        | 1.4             |
| 1Q8N  | 6.1          | 5.0   | 0.4        | 0.4             |
| 1TOB  | 5.3          | 5.3   | 2.6        | 2.6             |
| 1UTS  | 7.2          | 4.4   | 2.1        | 2.3             |
| 1UUD  | 3.4          | 4.0   | 3.0        | 2.6             |
| 1UUI  | 5.6          | 4.4   | 3.7        | 4.8             |
| 1XPF  | 3.7          | 3.2   | 3.8        | 4.0             |
| 2BE0  | 14.2         | 12.7  | no solutions found | no solutions found |
| 2BEE  | 10.8         | 10.9  | no solutions found | no solutions found |
| 2ET8  | 4.8          | 4.2   | 4.4        | 2.7             |
| 2F4U  | 6.2          | 6.0   | 5.0        | 5.6             |
| 2FCZ  | 8.9          | 7.3   | no solutions found | no solutions found |
| 2GDI  | 32.3         | 31.1  | 1.6        | 2.3             |
| 2O3X  | 4.3          | 4.1   | 4.9        | 4.3             |
| 2OE5  | 4.1          | 4.2   | 5.4        | 2.6             |
| 2PWT  | 19.1         | 19.6  | no solutions found | no solutions found |
| 2TOB  | 5.6          | 5.6   | 1.8        | 1.4             |
| 3D2X  | 12.1         | 10.8  | 2.5        | 1.8             |
| 3GX2  | 3.8          | 3.7   | 1.9        | 0.8             |
| 3SUX  | 2.6          | 0.9   | 0.7        | 0.8             |

A. All data (33 structures):

- Average: 7.1 (AutodockVina), 6.5 (iDock), 2.6 (rdock-dock), 2.3 (rdock-dock_solv)
- Median: 5.1 (AutodockVina), 4.4 (iDock), 2.1 (rdock-dock), 1.9 (rdock-dock_solv)

B. Docking completed for all four docking programs (29 structures):

- Average: 6.2 (AutodockVina), 5.6 (iDock), 2.6 (rdock-dock), 2.3 (rdock-dock_solv)
- Median: 4.8 (AutodockVina), 4.2 (iDock), 2.1 (rdock-dock), 1.9 (rdock-dock_solv)

C. Docking completed for all four docking programs and all RMSD values < 10 Å (25 structures):

- Average: 4.4 (AutodockVina), 4.0 (iDock), 2.4 (rdock-dock), 2.2 (rdock-dock_solv)
- Median: 4.6 (AutodockVina), 4.2 (iDock), 1.9 (rdock-dock), 1.4 (rdock-dock_solv)
