

## Lead-Finder docking test set composition

| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 121p   | 1.54 | 8                | 1           | 1.29      | 0.71         |              |          |          |          |               |             |             |
| 186l   | 1.8  | 3                | 1           |           |              |              |          |          |          | 1             |             |             |
| 1a28   | 1.8  | 1                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1a4q   | 1.9  | 8                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1a6w   | 1.8  | 4                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1a9u   | 2.5  | 3                | 1           |           |              |              |          |          |          | 1             |             |             |
| 1aaq   | 2.5  | 17               | 1           | 1.29      | 1.40         | 2.01         | 1        |          |          |               |             |             |
| 1abe   | 1.7  | 0                | 1           | 1.16      | 0.40         | 0.31         | 1        |          | 1        | 1             | 0.26        | 0.27        |
| 1abf   | 1.9  | 0                | 1           | 1.16      | 0.14         | 0.17         |          |          | 1        |               |             |             |
| 1acj   | 2.8  | 0                | 1           | 0.49      | 4.61         | 2.81         | 1        |          |          |               | 0.78        | 3.89        |
| 1ack   | 2.8  | 2                | 1           |           |              |              |          |          |          | 1             |             | 1.18        |
| 1acl   | 2.8  | 11               | 0           |           |              |              | 1        |          |          |               |             |             |
| 1acm   | 2.8  | 6                | 1           | 0.49      | 0.32         | 0.40         | 1        |          |          | 1             | 0.56        | 1.43        |
| 1aco   | 2.05 | 4                | 1           | 0.96      | 0.29         | 0.34         | 1        |          |          | 1             | 0.42        | 3.39        |
| 1add   | 2.4  | 2                | 1           |           | 0.70         | 0.83         |          |          |          |               |             |             |
| 1adf   | 2.9  | 10               | 0           |           | 9.92         | 3.03         |          |          |          |               |             |             |
| 1aec   | 1.86 | 13               | 1           |           |              |              | 1        |          | 1        | 1             |             |             |
| 1aha   | 2.2  | 0                | 1           | 0.96      | 0.11         | 0.36         | 1        |          |          | 1             | 0.32        | 0.37        |
| 1ake   | 1.9  | 16               | 0           | 1.18      | 14.95        | 15.45        |          |          |          |               |             |             |
| 1aoe   | 1.6  | 3                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1apb   | 1.76 | 0                | 1           |           | 0.10         | 0.06         |          |          |          |               |             |             |
| 1apt   | 1.8  | 17               | 0           | 1.18      | 1.24         | 1.48         | 1        |          | 1        | 1             |             |             |
| 1apu   | 1.8  | 14               | 0           |           | 1.24         | 0.61         |          |          | 1        |               |             |             |
| 1apv   | 1.8  | 14               | 1           |           | 0.48         | 0.63         |          |          |          |               |             |             |
| 1apw   | 1.8  | 14               | 0           |           | 0.32         | 0.97         |          |          |          |               |             |             |
| 1aqw   | 1.8  | 9                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1ase   | 2.5  | 5                | 1           |           |              |              | 1        |          |          | 1             |             |             |
| 1atl   | 1.8  | 9                | 1           | 2.06      | 3.47         | 0.87         | 1        |          | 1        |               | 1.59        | 7.01        |
| 1avd   | 2.7  | 5                | 1           | 2.06      | 0.55         | 0.82         |          |          |          |               |             |             |
| 1azm   | 2    | 1                | 1           | 2.37      | 2.51         | 1.89         | 1        |          |          | 1             |             |             |
| 1b40   | 2.2  | 15               | 1           |           |              |              |          |          |          | 1             |             |             |
| 1b58   | 1.8  | 15               | 1           |           |              |              |          |          | 1        |               |             |             |
| 1b59   | 1.8  | 6                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1b6j   | 1.85 | 13               | 1           |           | 0.43         | 2.98         |          |          |          |               |             |             |
| 1b6k   | 1.85 | 12               | 1           |           | 1.06         | 1.04         |          |          |          |               |             |             |
| 1b6l   | 1.75 | 7                | 1           |           | 1.18         | 0.92         |          |          |          |               |             |             |
| 1b6m   | 1.85 | 11               | 1           |           | 3.17         | 0.73         |          |          |          |               |             |             |
| 1baf   | 2.9  | 5                | 0           | 2.37      | 1.08         | 1.17         | 1        |          |          | 1             | 1.6         | 6.52        |
| 1bap   | 1.75 | 0                | 1           |           | 0.38         | 0.39         |          |          |          |               |             |             |
| 1bbp   | 2    | 8                | 1           | 3.75      | 5.11         | 5.28         | 1        |          |          |               | 0.99        | 1.07        |
| 1bkm   | 2    | 16               | 0           |           | 2.36         | 4.77         |          |          |          |               |             |             |
| 1blh   | 2.3  | 6                | 1           |           |              |              | 1        |          |          | 1             |             |             |
| 1bma   | 1.8  | 12               | 1           | 3.75      | 1.94         | 0.68         | 1        |          | 1        |               | 1.04        | 3           |
| 1bra   | 2.2  | 0                | 1           |           | 0.32         | 2.26         |          |          |          |               |             |             |
| 1byb   | 1.9  | 10               | 1           | 1.62      | 0.46         | 0.56         | 1        |          | 1        |               |             |             |
| 1c1b   | 2.5  | 6                | 1           |           | 0.45         | 0.91         |          |          |          |               |             |             |
| 1c1e   | 1.9  | 0                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1c3i   | 1.83 | 12               | 1           |           | 0.43         | 0.61         |          |          |          |               |             |             |
| 1c5c   | 1.61 | 0                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1c5p   | 1.43 | 0                | 1           |           | 0.25         | 0.27         |          |          |          |               |             |             |
| 1c5x   | 1.75 | 0                | 1           |           |              |              |          |          | 1        |               |             |             |

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|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1c83   | 1.8  | 2                | 1           |           | 0.14         | 0.17         |          |          | 1        |               |             |             |
| 1c84   | 2.35 | 2                | 1           |           | 0.32         | 0.26         |          |          |          |               |             |             |
| 1c86   | 2.3  | 2                | 1           |           | 0.18         | 0.19         |          |          |          |               |             |             |
| 1c87   | 2.1  | 2                | 1           |           | 0.21         | 0.28         |          |          |          |               |             |             |
| 1c88   | 1.8  | 2                | 1           |           | 0.22         | 0.25         |          |          |          |               |             |             |
| 1c8k   | 1.76 | 2                | 0           |           | 5.50         | 3.28         |          |          |          |               |             |             |
| 1cbs   | 1.8  | 1                | 1           | 1.62      | 0.39         | 0.63         | 1        |          | 1        |               | 1.43        | 1.77        |
| 1cbx   | 2    | 5                | 1           | 1.35      | 0.48         | 0.28         | 1        |          |          | 1             | 1.06        | 0.7         |
| 1cde   | 2.5  | 5                | 1           | 1.35      | 1.71         | 1.62         |          |          |          |               |             |             |
| 1cdg   | 2    | 4                | 1           | 4.87      | 9.83         | 6.48         | 1        |          |          |               |             |             |
| 1cil   | 1.6  | 3                | 1           | 4.87      | 3.92         | 3.61         | 1        |          | 1        |               |             |             |
| 1cnx   | 1.9  | 9                | 0           |           | 6.53         | 6.54         |          |          |          |               |             |             |
| 1com   | 2.2  | 4                | 1           | 1.62      | 3.74         | 0.55         | 1        |          |          |               | 0.75        | 0.86        |
| 1coy   | 1.8  | 0                | 1           | 1.62      | 0.29         | 0.44         | 1        |          | 1        | 1             | 0.66        | 0.54        |
| 1cps   | 2.25 | 5                | 1           | 0.99      | 1.29         |              | 1        |          |          |               |             |             |
| 1ctr   | 2.45 | 5                | 0           | 0.99      | 2.59         | 2.27         | 1        |          |          |               |             |             |
| 1ctt   | 2.2  | 2                | 1           |           | 5.04         | 0.60         |          |          |          |               |             |             |
| 1d0l   | 1.97 | 11               | 1           |           |              |              |          |          | 1        |               |             |             |
| 1d3d   | 2.04 | 9                | 0           |           | 2.74         | 1.52         |          |          |          |               |             |             |
| 1d3h   | 1.8  | 4                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1d3p   | 2.1  | 11               | 0           |           | 2.05         | 1.72         |          |          |          |               |             |             |
| 1d7x   | 2    | 5                | 1           |           | 0.44         | 0.58         |          |          |          |               |             |             |
| 1d8f   | 2.4  | 6                | 1           |           | 4.31         | 4.25         |          |          |          |               |             |             |
| 1dbb   | 2.7  | 1                | 1           | 0.81      | 0.41         | 0.37         | 1        |          |          | 1             | 1.62        | 0.54        |
| 1dbj   | 2.7  | 0                | 1           | 0.81      | 0.21         | 0.32         | 1        |          |          | 1             | 0.93        | 3           |
| 1dbk   | 3    | 0                | 1           | 0.76      | 0.40         | 0.57         |          |          |          |               |             |             |
| 1dbm   | 2.7  | 6                | 1           | 0.76      | 1.97         | 1.95         |          |          |          |               |             |             |
| 1dd6   | 2    | 9                | 1           |           | 8.27         | 1.36         |          |          |          |               |             |             |
| 1dds   | 2.2  | 7                | 1           |           | 2.38         | 1.75         |          |          |          |               |             |             |
| 1dhf   | 2.3  | 5                | 1           |           | 5.62         | 6.31         |          |          |          |               |             |             |
| 1did   | 2.5  | 2                | 1           | 4.22      | 4.15         | 3.27         | 1        |          |          |               |             |             |
| 1die   | 2.5  | 1                | 1           | 4.22      | 0.77         | 0.34         | 1        |          |          |               |             |             |
| 1dih   | 2.2  | 12               | 0           |           | 1.78         | 2.62         |          |          |          |               |             |             |
| 1dm2   | 2.1  | 0                | 1           |           | 0.69         | 0.66         |          |          |          |               |             |             |
| 1dog   | 2.4  | 1                | 1           |           | 3.77         | 3.77         |          |          |          |               |             |             |
| 1dr1   | 2.2  | 2                | 1           | 5.64      | 1.46         | 0.37         | 1        |          |          |               | 0.65        | 1.25        |
| 1dwb   | 3.16 | 0                | 1           | 5.64      | 0.32         | 0.29         |          |          |          |               |             |             |
| 1dwc   | 3    | 8                | 1           | 1.19      | 0.89         | 2.06         |          |          |          |               |             |             |
| 1dwd   | 3    | 7                | 1           | 1.19      | 1.43         | 0.47         | 1        |          |          |               | 1.07        | 1.68        |
| 1e5i   | 2.1  | 4                | 0           |           | 0.17         | 0.28         |          |          |          |               |             |             |
| 1eap   | 2.5  | 10               | 1           | 3.72      | 2.38         | 0.65         | 1        |          |          | 1             | 2.52        | 4.89        |
| 1ebg   | 2.1  | 2                | 1           |           | 0.26         | 0.34         |          |          |          |               |             |             |
| 1ecv   | 1.95 | 2                | 1           |           | 0.18         | 0.24         |          |          |          |               |             |             |
| 1eed   | 2    | 19               | 0           | 3.72      | 1.58         | 11.29        | 1        |          |          | 1             |             |             |
| 1ejn   | 1.8  | 4                | 1           |           | 0.12         | 0.34         |          |          | 1        |               |             |             |
| 1ela   | 1.8  | 9                | 1           | 9.71      | 6.01         | 0.39         |          |          |          |               |             |             |
| 1elb   | 2.1  | 13               | 0           | 9.71      | 4.29         | 5.42         |          |          |          |               |             |             |
| 1elc   | 1.75 | 13               | 0           | 4.74      | 7.92         | 6.53         |          |          |          |               |             |             |
| 1eld   | 1.8  | 8                | 1           | 4.74      | 3.94         | 0.32         |          |          |          |               |             |             |
| 1ele   | 1.8  | 7                | 1           | 10.73     | 0.38         | 0.36         |          |          |          |               |             |             |
| 1epb   | 2.2  | 1                | 1           | 10.73     | 1.89         | 2.24         | 1        |          |          | 1             | 3.35        | 2.87        |

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|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1eta   | 1.7  | 5                | 1           | 8.46      | 1.85         | 8.69         | 1        |          | 1        | 1             |             |             |
| 1etr   | 2.2  | 8                | 1           | 8.46      | 0.68         | 0.71         | 1        |          |          | 1             | 1.96        | 4.05        |
| 1ets   | 2.3  | 7                | 1           |           | 1.44         | 1.32         |          |          |          |               |             |             |
| 1ett   | 2.5  | 5                | 1           |           | 0.58         | 0.62         |          |          |          |               |             |             |
| 1ezq   | 2.2  | 8                | 1           |           | 0.21         | 0.75         |          |          |          |               |             |             |
| 1f0r   | 2.1  | 4                | 1           |           | 0.59         | 2.11         |          |          |          |               |             |             |
| 1f0s   | 2.1  | 4                | 1           |           | 0.35         | 2.08         |          |          |          |               |             |             |
| 1f0t   | 1.8  | 4                | 1           |           | 0.24         | 0.38         |          |          |          |               |             |             |
| 1f0u   | 1.9  | 8                | 1           |           | 1.54         | 1.56         |          |          |          |               |             |             |
| 1f3d   | 1.87 | 2                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1fen   | 1.9  | 1                | 1           | 1.39      | 0.40         | 1.10         | 1        |          | 1        |               | 0.89        | 1.18        |
| 1fh8   | 1.95 | 2                | 1           |           | 0.20         | 0.20         |          |          |          |               |             |             |
| 1fh9   | 1.72 | 2                | 1           |           | 1.99         | 2.11         |          |          |          |               |             |             |
| 1fhd   | 1.9  | 2                | 1           |           | 0.46         | 5.37         |          |          |          |               |             |             |
| 1fjs   | 1.92 | 8                | 0           |           | 2.42         | 2.06         |          |          |          |               |             |             |
| 1fkg   | 2    | 10               | 1           | 1.39      | 1.33         | 1.21         | 1        |          |          | 1             | 1.89        | 3           |
| 1fki   | 2.2  | 0                | 1           | 0.59      | 1.29         | 1.30         | 1        |          |          |               | 0.84        | 0.7         |
| 1flr   | 1.85 | 2                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1fq5   | 2.4  | 10               | 1           |           | 2.43         | 1.96         |          |          |          |               |             |             |
| 1frp   | 2    | 4                | 1           | 0.59      | 0.27         |              | 1        |          |          |               | 0.92        | 0.75        |
| 1fmt   | 2.2  | 2                | 1           |           | 0.88         | 0.88         |          |          |          |               |             |             |
| 1g45   | 1.83 | 3                | 0           |           | 4.02         | 7.88         |          |          |          |               |             |             |
| 1g46   | 1.84 | 3                | 0           |           | 4.50         | 8.06         |          |          |          |               |             |             |
| 1g48   | 1.86 | 3                | 0           |           | 3.77         | 1.88         |          |          |          |               |             |             |
| 1g4j   | 1.84 | 3                | 1           |           | 3.51         | 5.56         |          |          |          |               |             |             |
| 1g4o   | 1.96 | 3                | 0           |           | 4.21         | 3.39         |          |          |          |               |             |             |
| 1g52   | 1.8  | 3                | 0           |           | 4.26         | 8.01         |          |          |          |               |             |             |
| 1g53   | 1.94 | 3                | 0           |           | 4.53         | 7.88         |          |          |          |               |             |             |
| 1g54   | 1.86 | 3                | 0           |           | 5.14         | 8.45         |          |          |          |               |             |             |
| 1g9v   | 1.85 | 6                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1ghb   | 2    | 4                | 1           | 1.33      | 0.30         | 0.45         | 1        |          |          | 1             |             |             |
| 1gkc   | 2.3  | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1glp   | 1.9  | 10               | 1           | 1.33      | 0.32         | 0.75         | 1        |          | 1        |               |             |             |
| 1glq   | 1.8  | 13               | 0           | 6.43      | 0.32         | 0.46         | 1        |          | 1        | 1             | 7.09        | 5.68        |
| 1gm8   | 2    | 4                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1gpk   | 2.1  | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1gsp   | 2.2  | 2                | 1           |           | 2.79         | 1.10         |          |          |          |               |             |             |
| 1hbv   | 2.3  | 14               | 1           |           | 2.07         | 2.19         |          |          |          |               |             |             |
| 1hdc   | 2.2  | 6                | 1           | 6.43      | 0.35         | 0.56         | 1        |          |          | 1             | 1.71        | 1.8         |
| 1hdy   | 2.5  | 0                | 1           | n/a       | 1.70         | 1.65         | 1        |          |          | 1             | 1.73        | 0.66        |
| 1hef   | 2.2  | 19               | 0           | n/a       | 6.43         | 6.24         | 1        |          |          |               |             |             |
| 1hfc   | 1.5  | 9                | 1           | 2.51      | 2.26         | 2.25         | 1        |          | 1        |               |             |             |
| 1hgg   | 2.9  | 3                | 1           | 2.51      | 1.47         | 1.37         |          |          |          |               |             |             |
| 1hgh   | 2.7  | 3                | 1           | 4.14      | 0.49         | 4.70         |          |          |          |               |             |             |
| 1hgi   | 2.7  | 3                | 1           | 4.14      | 0.23         | 0.37         |          |          |          |               |             |             |
| 1hgj   | 2.7  | 3                | 1           | 3.98      | 0.34         | 0.64         |          |          |          |               |             |             |
| 1hih   | 2.2  | 15               | 1           |           | 1.29         | 1.26         |          |          |          |               |             |             |
| 1hnn   | 2.4  | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hp0   | 2.1  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hps   | 2.3  | 16               | 1           |           | 2.09         | 11.93        |          |          |          |               |             |             |
| 1hpv   | 1.9  | 11               | 1           |           | 0.93         | 1.05         |          |          | 1        |               |             |             |

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|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1hpx   | 2    | 14               | 0           |           | 3.31         | 3.34         |          |          |          |               |             |             |
| 1hq2   | 1.25 | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hri   | 3    | 9                | 1           | 3.98      | 2.26         | 10.09        | 1        |          |          | 1             | 6.33        | 1.98        |
| 1hsb   | 1.9  | 7                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1hsg   | 2    | 12               | 1           |           | 0.35         | 0.41         |          |          |          |               |             |             |
| 1hsl   | 1.89 | 3                | 1           | 0.59      | 1.31         | 1.31         | 1        |          | 1        | 1             | 0.49        | 0.51        |
| 1hte   | 2.8  | 8                | 0           |           | 7.36         | 7.32         |          |          |          |               |             |             |
| 1htf   | 2.2  | 12               | 0           |           | 2.74         | 2.19         |          |          |          |               |             |             |
| 1hti   | 2.8  | 3                | 1           | 0.59      | 1.60         | 4.40         |          |          |          |               |             |             |
| 1hvr   | 1.8  | 8                | 1           | 3.35      | 1.75         | 1.60         |          |          | 1        |               |             |             |
| 1hvy   | 1.9  | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hwi   | 2.3  | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hww   | 1.87 | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1hyt   | 1.7  | 5                | 1           | 3.35      | 0.43         | 2.65         | 1        |          | 1        | 1             | 1.61        | 3           |
| 1ia1   | 1.7  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1icn   | 1.74 | 15               | 0           | 10.52     | 2.04         | 9.06         | 1        |          |          | 1             |             |             |
| 1ida   | 1.7  | 14               | 1           | 10.52     | 2.12         | 1.95         | 1        |          | 1        | 1             |             |             |
| 1ig3   | 1.9  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1igj   | 2.5  | 3                | 1           | 7.17      | 0.46         | 0.72         | 1        |          |          | 1             |             |             |
| 1imb   | 2.2  | 2                | 0           | 7.17      | 1.64         | 1.84         | 1        |          |          |               |             |             |
| 1ivb   | 2.4  | 3                | 1           | 1.29      | 0.47         | 3.27         |          |          |          |               |             |             |
| 1ivc   | 2.4  | 1                | 1           | 1.29      | 1.89         | 2.05         |          |          |          |               |             |             |
| 1ivd   | 1.9  | 3                | 0           | 5.42      | 0.73         | 0.73         |          |          |          |               |             |             |
| 1ive   | 2.4  | 2                | 1           | 5.42      | 5.17         | 5.11         | 1        |          |          | 1             |             |             |
| 1ivf   | 2.4  | 5                | 1           | 6.97      | 0.59         | 0.61         |          |          |          |               |             |             |
| 1j3j   | 2.3  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1jap   | 1.82 | 7                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1jd0   | 1.5  | 1                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1jje   | 1.8  | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1jla   | 2.5  | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1k3u   | 1.7  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1ke5   | 2.2  | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1kel   | 1.9  | 10               | 1           |           |              |              |          |          | 1        |               |             |             |
| 1kzk   | 1.09 | 9                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1l2s   | 1.94 | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1l7f   | 1.8  | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1lah   | 2.06 | 4                | 1           | 6.97      | 0.19         | 0.52         | 1        |          |          |               | 0.32        | 0.3         |
| 1lcp   | 1.65 | 3                | 1           | 1.65      | 1.06         | 1.82         | 1        |          | 1        |               | 1.59        | 2.01        |
| 1ldm   | 2.1  | 1                | 1           | 1.65      | 1.35         | 1.34         | 1        |          |          | 1             | 0.73        | 0.44        |
| 1lic   | 1.6  | 15               | 1           | 5.07      | 4.99         | 3.96         | 1        |          | 1        | 1             | 2.44        | 3.46        |
| 1lmo   | 1.8  | 6                | 0           | 5.07      | 0.87         | 8.40         | 1        |          |          |               |             |             |
| 1lna   | 1.9  | 8                | 1           | 5.4       | 0.90         | 1.50         | 1        |          | 1        |               | 3.04        | 0.88        |
| 1lpm   | 2.18 | 9                | 1           |           |              |              | 1        |          |          |               |             | 1.87        |
| 1lpz   | 2.4  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1lrh   | 1.9  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1lst   | 1.8  | 5                | 1           | 5.4       | 0.27         | 0.75         | 1        |          | 1        | 1             | 0.23        | 0.33        |
| 1m2z   | 2.5  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1mbi   | 2    | 0                | 1           | 0.47      | 1.65         | 1.92         |          |          |          |               |             |             |
| 1mcr   | 2.7  | 5                | 1           | 0.47      | 4.33         | 5.82         | 1        |          |          | 1             |             |             |
| 1mdr   | 2.1  | 2                | 1           | 0.88      | 0.54         | 1.95         | 1        |          |          | 1             | 1.09        | 0.68        |
| 1meh   | 1.95 | 6                | 0           |           |              |              |          | 1        |          |               |             |             |

## Lead-Finder docking test set composition

| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1mfe   | 2    | 6                | 0           |           | 1.78         | 6.09         |          |          |          |               |             |             |
| 1mld   | 1.83 | 5                | 1           | 0.88      | 0.22         | 0.25         |          |          | 1        |               |             |             |
| 1mmq   | 1.9  | 6                | 1           | 0.52      | 0.33         | 0.67         | 1        |          | 1        |               |             |             |
| 1mmv   | 2    | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1mnc   | 2.1  | 9                | 1           |           | 0.73         | 0.33         |          |          |          |               |             |             |
| 1mrg   | 1.8  | 0                | 1           | 0.52      | 0.12         | 0.15         | 1        |          | 1        |               | 0.45        | 0.7         |
| 1mrk   | 1.6  | 2                | 1           | 3.55      | 1.17         | 1.21         | 1        |          | 1        | 1             | 1.37        | 0.85        |
| 1mts   | 1.9  | 6                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1mup   | 2.4  | 2                | 1           | 3.55      | 4.05         | 4.50         | 1        |          |          | 1             |             |             |
| 1mzc   | 2    | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1n1m   | 2.5  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1n2j   | 1.8  | 3                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1n2v   | 2.1  | 3                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1n46   | 2.2  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1nav   | 2.5  | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1nco   | 1.8  | 8                | 1           | 5.85      | 0.33         | 0.60         | 1        |          | 1        |               | 0.39        | 8.26        |
| 1nis   | 2.05 | 5                | 1           | 5.85      | 0.45         | 0.26         | 1        |          |          |               |             |             |
| 1nnb   | 2.8  | 5                | 1           |           | 0.25         | 1.39         |          |          |          |               |             |             |
| 1nsc   | 1.7  | 5                | 1           | 2.12      | 0.24         | 0.66         |          |          |          |               |             |             |
| 1nsd   | 1.8  | 5                | 1           |           | 0.22         | 0.74         |          |          |          |               |             |             |
| 1odw   | 2.1  | 16               | 1           |           | 2.59         | 3.91         |          |          |          |               |             |             |
| 1of1   | 1.95 | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1of6   | 2.1  | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1okl   | 2.1  | 2                | 1           |           | 3.14         | 0.38         |          |          |          |               |             |             |
| 1opk   | 1.8  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1oq5   | 1.5  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1owe   | 1.6  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1oyt   | 1.67 | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1p2y   | 2.3  | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1p62   | 1.9  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1pbd   | 2.3  | 1                | 1           | 2.12      | 0.26         | 0.32         | 1        |          |          | 1             |             |             |
| 1pgp   | 2.5  | 7                | 1           |           | 1.83         | 2.23         |          |          |          |               |             |             |
| 1pha   | 1.63 | 8                | 1           | n/a       | 0.52         | 1.04         | 1        |          |          |               |             |             |
| 1phd   | 1.6  | 1                | 1           | 0.65      | 0.30         | 1.13         | 1        |          | 1        | 1             |             |             |
| 1phf   | 1.6  | 1                | 1           | 4.23      | 1.11         | 1.46         |          |          |          |               |             |             |
| 1phg   | 1.6  | 3                | 1           | 4.23      | 1.20         | 4.29         | 1        |          | 1        |               | 1.38        | 4.44        |
| 1pmn   | 2.2  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1poc   | 2    | 23               | 0           | 9.25      | 1.52         | 1.44         | 1        |          |          | 1             |             |             |
| 1ppc   | 1.8  | 7                | 1           | 9.25      | 6.31         | 1.40         |          |          | 1        |               |             |             |
| 1pph   | 1.9  | 5                | 1           | 4.91      | 0.58         | 0.70         |          |          | 1        |               |             |             |
| 1ppi   | 2.2  | 11               | 0           | 4.91      | 2.80         | 1.01         |          |          |          |               |             |             |
| 1ppk   | 1.8  | 14               | 1           | 1.54      | 0.27         | 0.73         |          |          |          |               |             |             |
| 1ppl   | 1.7  | 18               | 1           | 1.54      | 2.55         | 0.70         |          |          |          |               |             |             |
| 1ppm   | 1.7  | 17               | 0           | 8.27      | 0.62         | 0.99         |          |          |          |               |             |             |
| 1pro   | 1.8  | 10               | 1           |           | 1.51         | 1.50         |          |          |          |               |             |             |
| 1pso   | 2    | 22               | 0           | 8.27      | 6.12         | 5.15         |          |          |          |               |             |             |
| 1q1g   | 2.02 | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1q41   | 2.1  | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1q4g   | 2    | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1qbr   | 1.8  | 6                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1qbu   | 1.8  | 8                | 1           |           |              |              |          |          | 1        |               |             |             |

## Lead-Finder docking test set composition

| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1r1h   | 1.95 | 9                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1r55   | 1.58 | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1r58   | 1.9  | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1r9o   | 2    | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1rbp   | 2    | 2                | 1           | 1.13      | 0.87         |              |          |          |          |               |             |             |
| 1rds   | 1.8  | 8                | 1           | 1.13      | 0.82         |              | 1        |          | 1        | 1             | 4.34        | 9.83        |
| 1rhl   | 1.95 | 4                | 1           |           | 0.42         |              |          |          |          |               |             |             |
| 1rls   | 1.9  | 4                | 1           |           | 0.51         |              |          |          |          |               |             |             |
| 1rne   | 2.4  | 21               | 1           | 12.24     | 3.51         |              | 1        |          |          | 1             |             |             |
| 1rnt   | 1.9  | 4                | 1           | 12.24     | 0.53         |              |          |          | 1        |               |             |             |
| 1rob   | 1.6  | 4                | 1           | 7.7       | 1.12         |              | 1        |          | 1        | 1             | 1.13        | 0.82        |
| 1s19   | 2.1  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1s3v   | 1.8  | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1sbg   | 2.3  | 14               | 1           |           | 0.40         | 0.88         |          |          |          |               |             |             |
| 1sbp   | 1.7  | 0                | 1           |           | 0.08         |              |          |          |          |               |             |             |
| 1sg0   | 1.5  | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1sj0   | 1.9  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1slt   | 1.9  | 5                | 1           | 7.7       | 0.57         | 1.03         | 1        |          | 1        | 1             |             |             |
| 1snc   | 1.65 | 6                | 1           | 7.48      | 1.12         | 2.06         | 1        |          | 1        |               | 1.69        | 4.92        |
| 1sq5   | 2.2  | 6                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1sqn   | 1.45 | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1sre   | 1.78 | 1                | 1           |           | 0.36         | 0.30         |          |          |          |               |             |             |
| 1srj   | 1.8  | 1                | 1           | 7.48      | 0.49         | 0.47         | 1        |          | 1        |               | 0.44        | 0.39        |
| 1stp   | 2.6  | 5                | 1           | 0.65      | 0.58         | 0.60         | 1        |          |          | 1             | 0.76        | 0.51        |
| 1t40   | 1.8  | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1t46   | 1.6  | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1t9b   | 2.2  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1tdb   | 2.65 | 4                | 1           | 0.65      | 7.50         | 7.34         | 1        |          |          | 1             |             |             |
| 1thy   | 2.9  | 4                | 1           | 2.67      | 4.21         | 1.98         |          |          |          |               |             |             |
| 1tka   | 2.7  | 8                | 1           | 2.67      | 2.28         | 2.28         | 1        |          |          | 1             | 1.35        | 1.96        |
| 1tlp   | 2.3  | 11               | 0           | 2.85      | 7.33         | 7.70         |          |          |          |               |             |             |
| 1tmn   | 1.9  | 13               | 1           | 2.85      | 1.90         | 3.65         | 1        |          | 1        |               | 5.58        | 1.3         |
| 1tng   | 1.8  | 1                | 1           | 1.93      | 0.21         | 0.26         | 1        |          | 1        |               | 0.51        | 0.22        |
| 1tnh   | 1.8  | 1                | 1           | 1.93      | 0.28         | 0.39         |          |          | 1        |               |             |             |
| 1tni   | 1.9  | 4                | 0           | 2.71      | 2.03         | 2.12         | 1        |          | 1        |               | 1.28        | 2.97        |
| 1tnj   | 1.8  | 2                | 1           | 2.71      | 0.36         | 0.43         |          |          |          |               |             |             |
| 1tnk   | 1.8  | 3                | 1           | 1.41      | 0.98         | 1.17         |          |          |          |               |             |             |
| 1tnl   | 1.9  | 1                | 1           | 1.41      | 0.24         | 0.54         | 1        |          | 1        |               | 0.46        | 2.26        |
| 1tow   | 2    | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1tph   | 1.8  | 3                | 1           | 1.5       | 0.23         | 0.22         | 1        |          |          |               |             |             |
| 1tpp   | 1.4  | 4                | 1           | 1.5       | 1.07         | 0.43         | 1        |          | 1        | 1             |             |             |
| 1trk   | 2    | 8                | 1           | 1.57      | 2.15         | 1.63         | 1        |          |          |               | 0.73        | 1.22        |
| 1tt1   | 1.93 | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1tyl   | 1.9  | 1                | 1           | 1.57      | 1.08         | 5.20         | 1        |          | 1        |               |             |             |
| 1tz8   | 1.85 | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1u1c   | 2.2  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1u4d   | 2.1  | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1ukz   | 1.9  | 4                | 1           | 0.94      | 0.41         | 0.55         | 1        |          | 1        |               | 0.36        | 0.77        |
| 1ulb   | 2.75 | 0                | 1           | 0.94      | 0.35         | 0.34         | 1        |          |          | 1             | 0.68        | 0.77        |
| 1uml   | 2.5  | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1unl   | 2.2  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |

## Lead-Finder docking test set composition

| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 1uou   | 2.11 | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1v0p   | 2    | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1v48   | 2.2  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1v4s   | 2.3  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1vcj   | 2.4  | 7                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1vgc   | 1.9  | 5                | 1           |           |              |              |          |          | 1        |               |             |             |
| 1w1p   | 2.1  | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1w2g   | 2.1  | 2                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1wap   | 1.8  | 3                | 1           | 0.57      | 0.19         | 0.23         | 1        |          | 1        |               | 0.48        | 0.3         |
| 1x8x   | 2    | 3                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1xid   | 1.7  | 2                | 1           | 0.57      | 4.32         | 4.02         | 1        |          | 1        |               |             |             |
| 1xie   | 1.7  | 1                | 1           | 1.94      | 3.91         | 2.60         | 1        |          | 1        | 1             |             |             |
| 1xm6   | 1.92 | 5                | 0           |           |              |              |          | 1        |          |               |             |             |
| 1xoq   | 1.83 | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1xoz   | 1.37 | 1                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1y6b   | 2.1  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1ygc   | 2    | 8                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1yqy   | 2.3  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1yv3   | 2    | 0                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1yvf   | 2.5  | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1ywr   | 1.95 | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 1z95   | 1.8  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 2ack   | 2.4  | 2                | 1           | 1.94      | 0.88         | 1.07         | 1        |          |          |               |             |             |
| 2ada   | 2.4  | 2                | 1           | 0.67      | 0.46         | 0.59         | 1        |          |          | 1             | 0.55        | 0.32        |
| 2ak3   | 1.85 | 4                | 1           | 0.67      | 0.70         |              | 1        |          | 1        | 1             | 0.49        | 0.6         |
| 2bm2   | 2.2  | 6                | 1           |           |              |              |          | 1        |          |               |             |             |
| 2br1   | 2    | 5                | 1           |           |              |              |          | 1        |          |               |             |             |
| 2bsm   | 2.05 | 4                | 1           |           |              |              |          | 1        |          |               |             |             |
| 2cgr   | 2.2  | 7                | 1           | 3.53      | 0.52         | 0.56         | 1        |          |          | 1             | 0.92        | 1.63        |
| 2cht   | 2.2  | 2                | 1           | 3.53      | 0.51         | 0.48         | 1        |          |          | 1             | 0.43        | 0.42        |
| 2cmd   | 1.87 | 5                | 1           | 3.75      | 0.34         | 0.65         | 1        |          | 1        |               | 0.5         | 1.6         |
| 2cpp   | 1.63 | 0                | 1           | 3.75      | 3.04         | 0.15         |          |          | 1        |               |             |             |
| 2ctc   | 1.4  | 3                | 1           | 1.97      | 1.58         | 1.43         | 1        |          | 1        |               | 0.37        | 0.38        |
| 2dbl   | 2.9  | 6                | 1           | 1.97      | 0.81         | 2.40         | 1        |          |          | 1             | 1.55        | 0.81        |
| 2er6   | 2    | 29               | 0           |           |              |              |          |          |          |               |             |             |
| 2fox   | 1.8  | 7                | 1           |           |              |              |          |          | 1        |               |             |             |
| 2gbp   | 1.9  | 1                | 1           | 0.92      | 0.14         | 0.61         | 1        |          | 1        |               | 0.36        | 0.63        |
| 2h4n   | 1.9  | 1                | 1           |           |              |              |          |          | 1        |               |             |             |
| 2ifb   | 2    | 14               | 1           |           | 1.77         | 2.27         |          |          |          |               |             |             |
| 2lgs   | 2.8  | 4                | 1           | 0.92      | 0.53         | 0.88         | 1        |          |          |               | 0.57        | 1.22        |
| 2mcp   | 3.1  | 4                | 1           | 2.07      | 1.25         | 1.54         | 1        |          |          | 1             |             |             |
| 2mth   | 1.9  | 2                | 1           |           |              |              |          |          |          |               |             |             |
| 2phh   | 2.7  | 1                | 1           | 2.07      | 0.41         | 0.47         | 1        |          |          | 1             | 0.69        | 3           |
| 2pk4   | 2.25 | 5                | 1           | 1.66      | 0.85         | 0.65         | 1        |          |          | 1             |             |             |
| 2plv   | 2.88 | 15               | 0           | 1.66      | 1.90         | 1.78         | 1        |          |          | 1             |             |             |
| 2qwk   | 1.8  | 6                | 1           |           |              |              |          |          | 1        |               |             |             |
| 2r04   | 3    | 9                | 1           | 12.55     | 0.75         | 1.44         |          |          |          |               |             |             |
| 2r07   | 3    | 7                | 1           | 12.55     | 0.67         | 0.92         | 1        |          |          | 1             | 1.81        | 1.35        |
| 2sim   | 1.6  | 5                | 1           | 1.99      | 0.94         | 0.82         | 1        |          |          | 1             | 1.29        | 1.1         |
| 2tmn   | 1.6  | 5                | 1           | 1.99      | 0.50         | 0.65         |          |          | 1        |               |             |             |
| 2tpi   | 2.1  | 6                | 1           |           | 1.15         | 0.26         |          |          |          |               |             |             |

## Lead-Finder docking test set composition

| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 2tsc   | 1.97 | 7                | 0           |           |              |              |          |          | 1        |               |             |             |
| 2upj   | 3    | 13               | 1           |           | 2.69         | 3.24         |          |          |          |               |             |             |
| 2xis   | 1.71 | 4                | 1           | 1.54      | 2.40         | 2.05         |          |          |          |               |             |             |
| 2yhx   | 2.1  | 3                | 1           | 1.54      | 2.19         | 1.91         | 1        |          |          | 1             |             |             |
| 2ypi   | 2.5  | 3                | 1           | 1.22      | 0.20         |              |          |          |          |               |             |             |
| 3aah   | 2.4  | 3                | 1           |           |              |              |          |          |          |               |             | 0.68        |
| 3cla   | 1.75 | 6                | 0           | 1.22      | 6.06         | 5.09         | 1        |          | 1        | 1             |             |             |
| 3cpa   | 2    | 5                | 1           | 2.53      | 0.66         |              | 1        |          |          |               | 1.63        | 1.9         |
| 3dfr   | 1.7  | 7                | 1           |           | 0.70         | 0.51         |          |          |          |               |             |             |
| 3ert   | 1.9  | 8                | 1           |           |              |              |          |          | 1        |               |             |             |
| 3gch   | 1.9  | 2                | 1           |           |              |              | 1        |          |          |               |             |             |
| 3hvt   | 2.9  | 1                | 1           | 2.53      | 0.79         | 0.72         | 1        |          |          | 1             | 0.35        | 1.64        |
| 3mth   | 1.9  | 2                | 0           | 1.59      | 5.62         | 1.23         | 1        |          |          |               |             |             |
| 3ptb   | 1.7  | 0                | 1           | 1.59      | 0.16         | 0.23         | 1        |          |          |               | 0.17        | 0.54        |
| 3tpi   | 1.9  | 6                | 1           | 1.07      | 0.51         | 0.47         | 1        |          | 1        |               | 0.36        | 0.52        |
| 4aah   | 2.4  | 3                | 1           | 1.07      | 0.24         | 0.25         | 1        |          |          | 1             |             |             |
| 4cts   | 2.9  | 3                | 1           | 1.53      | 0.19         | 0.25         | 1        |          |          | 1             | 0.6         | 2.2         |
| 4dfr   | 1.7  | 7                | 1           | 1.53      | 5.17         | 0.92         | 1        |          | 1        | 1             | 1.39        | 1.6         |
| 4est   | 1.78 | 13               | 0           |           |              |              | 1        |          | 1        | 1             |             |             |
| 4fab   | 2.7  | 2                | 1           | 4.95      | 0.82         | 4.44         | 1        |          |          | 1             |             |             |
| 4fbp   | 2.5  | 4                | 1           | 4.95      | 0.55         | 2.03         |          |          |          |               |             |             |
| 4fxn   | 0    | 7                | 1           | 1.04      | 0.49         | 0.50         |          |          |          |               |             |             |
| 4hmg   | 3    | 3                | 1           | 1.04      | 0.67         | 0.54         |          |          |          |               |             |             |
| 4phv   | 2.1  | 12               | 0           | 1.12      | 4.22         | 0.55         | 1        |          |          | 1             |             |             |
| 4tim   | 2.4  | 4                | 1           | 1.12      | 1.32         | 1.32         |          |          |          |               |             |             |
| 4tln   | 2.3  | 3                | 1           | 3.68      | 2.67         | 1.43         |          |          |          |               |             |             |
| 4tmn   | 1.7  | 14               | 0           | 3.68      | 0.73         | 1.29         |          |          |          |               |             |             |
| 4tpi   | 2.2  | 5                | 1           |           | 0.56         | 0.88         |          |          |          |               |             |             |
| 4ts1   | 2.5  | 3                | 1           | 1.41      | 0.85         | 0.89         |          |          |          |               |             |             |
| 5abp   | 1.8  | 1                | 1           | 1.41      | 0.20         | 0.11         |          |          | 1        |               |             |             |
| 5cpp   | 2.08 | 0                | 1           | 1.49      | 2.65         | 0.11         |          |          |          |               |             |             |
| 5cts   | 1.9  | 3                | 1           | 1.49      | 0.27         | 0.27         |          |          |          |               |             |             |
| 5p2p   | 2.4  | 20               | 1           | 1         | 6.18         | 4.95         | 1        |          |          |               |             |             |
| 5tim   | 1.83 | 0                | 0           | 1         | 0.69         | 1.32         |          |          |          |               |             |             |
| 5tln   | 2.3  | 8                | 1           |           | 1.01         | 2.37         |          |          |          |               |             |             |
| 5tmn   | 1.6  | 14               | 0           | 4.38      | 2.50         | 2.87         |          |          |          |               |             |             |
| 6abp   | 1.67 | 0                | 1           | 4.38      | 0.36         | 0.33         | 1        |          |          |               | 0.3         | 0.28        |
| 6cpa   | 2    | 12               | 1           | 6.61      | 4.29         | 3.93         |          |          |          |               |             |             |
| 6rnt   | 1.8  | 4                | 1           | 6.61      | 0.63         | 0.63         | 1        |          | 1        | 1             | 7.48        | 3           |
| 6rsa   | 2    | 2                | 1           |           |              |              | 1        |          |          |               |             | 0.78        |
| 6tim   | 2.2  | 4                | 1           | 1.6       | 0.42         | 0.59         |          |          |          |               |             |             |
| 6tmn   | 1.6  | 14               | 0           | 1.6       | 2.57         | 2.53         |          |          |          |               |             |             |
| 7abp   | 1.67 | 0                | 1           |           | 0.17         | 0.15         |          |          |          |               |             |             |
| 7cpa   | 2    | 15               | 1           | 9.11      | 2.87         | 3.91         |          |          |          |               |             |             |
| 7cpp   | 2    | 0                | 1           |           | 3.23         | 1.99         |          |          |          |               |             |             |
| 7tim   | 1.9  | 3                | 1           | 9.11      | 0.19         | 0.20         | 1        |          | 1        | 1             | 0.58        | 1.2         |
| 7upj   | 2    | 5                | 1           |           |              |              |          |          |          | 1             |             |             |
| 8abp   | 1.49 | 1                | 1           |           | 0.21         | 0.10         |          |          |          |               |             |             |
| 8atc   | 2.5  | 6                | 1           | 0.62      | 0.38         | 0.41         |          |          |          |               |             |             |
| 8gch   | 1.6  | 8                | 1           | 0.62      | 0.30         | 0.32         | 1        |          |          | 1             | 4.07        | 4.51        |
| 9abp   | 1.97 | 1                | 1           |           | 0.13         | 0.23         |          |          |          |               |             |             |



| PDB ID | R, Å | N <sub>frb</sub> | Lead-Finder | FlexX [1] | Glide SP [2] | Glide XP [3] | Gold [4] | Gold [5] | Gold [6] | LigandFit [7] | MolDock [8] | Surflex [9] |
|--------|------|------------------|-------------|-----------|--------------|--------------|----------|----------|----------|---------------|-------------|-------------|
| 9hvp   | 2.8  | 20               | 0           | 15.54     | 1.47         | 1.44         |          |          |          |               |             |             |

Composition of the entire test set of 407 protein-ligand complexes by original test sets of FlexX, Glide SP, Glide XP, Gold, LigandFit, MolDock, Surflex docking programs. Column 'PDBid' contains PDB codes of protein-ligand complexes, column 'R' – structure resolution in Å; column 'N<sub>FRB</sub>' – the number of freely rotatable ligand bonds. In the 'Lead-Finder' column successfully docked ligands are marked with '1', misdocked structures are marked with '0'. In columns corresponding to other docking programs RMSD (in Å) between the top-ranked and reference ligand pose are provided when corresponding data are available (from original publications); when such data are not available, only inclusion of particular protein-ligand complex in the test set is marked with '1'.

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