

Figure S1. Binding models and multiple sequence alignments of PPI family in Skp1-Skp2-Cks1 complex (PDB code 2ast). (A) The atomic binding model with hydrogen bonds (red dash lines) for each interface of the template. (B) Multiple sequence alignments of the interface B-C (Skp2-Cks1). This interface includes 11 and 26 homologous proteins of the chains B (Skp2) and C (Cks1), respectively.

A

| 1eerA side (Query 1) | | | | | | | | | |
|----------------------|-------|-----|----|------|------|----------|----------|-------------------|-------------------|
| 1eer-A | | | | 10 | 80 | 100 | 110 | | |
| | | | | APPR | ICDS | SVLERYLL | QALLV | DKAVSGLRSLTLLRAL | |
| Query 1 | | | | APPR | ICDS | SVLERYIL | QALLA | DKAISGLRSLTSLLRVL | |
| P01588 | 9606 | PRI | 28 | : | APPR | ICDS | SVLERYLL | QALLV | DKAVSGLRSLTLLRAL |
| P07321 | 10090 | ROD | 27 | : | APPR | ICDS | SVLERYIL | QALLA | DKAISGLRSLTSLLRVL |
| B7ZMY9 | 10090 | ROD | 27 | : | APPR | ICDS | SVLERYIL | QALLA | DKAISGLRSLTSLLRVL |
| P29676 | 10116 | ROD | 27 | : | APPR | ICDS | SVLERYIL | QALQA | DKAISGLRSLTSLLRVL |

B

| 1eerC side (Query 2) | | | | | | | | | | |
|----------------------|-------|-----|----|--------|--------|----------|----------|-------|-------|-------|
| 1eer-C | | | | 30 | 60 | 90 | 150 | 150 | 200 | |
| | | | | TERLED | LEDEP | TADTSSFV | PMTSH | PMTSH | MAEPS | |
| Query 2 | | | | TQRLED | LEGES | TADTSSFV | PMTH | PMTH | MAEPS | |
| P19235 | 9606 | PRI | 32 | : | TERLED | LEDEP | TADTSSFV | PMTSH | PMTSH | MAEPS |
| P14753 | 10090 | ROD | 32 | : | TQRLED | LEGES | TADTSSFV | PMTH | PMTH | MAEPS |
| O35545 | 10116 | ROD | 32 | : | TQRLED | LEGES | TADTSSFV | PMTH | PMTH | MAEPS |
| Q07303 | 10116 | ROD | 32 | : | TQRLED | LEGES | TADTSSFV | PMTH | PMTH | MAEPS |
| Q5FVS4 | 10116 | ROD | 32 | : | TQRLED | LEGES | TADTSSFV | PMTH | PMTH | MAEPS |

| Description | |
|----------------------|--|
| Template (structure) | Contact residues: Marked by 4 colors Hydrogen-bond residues: green Conserved residues: orange Both: yellow Others: gray |

Figure S2. Multiple sequence alignments of the (Epo-Epor) A-C interface of template cytokine/receptor complex (PDB code 1eer). This interface includes five and six homologous proteins of the chains A (erythropoietin) and C (erythropoietin receptors), respectively.

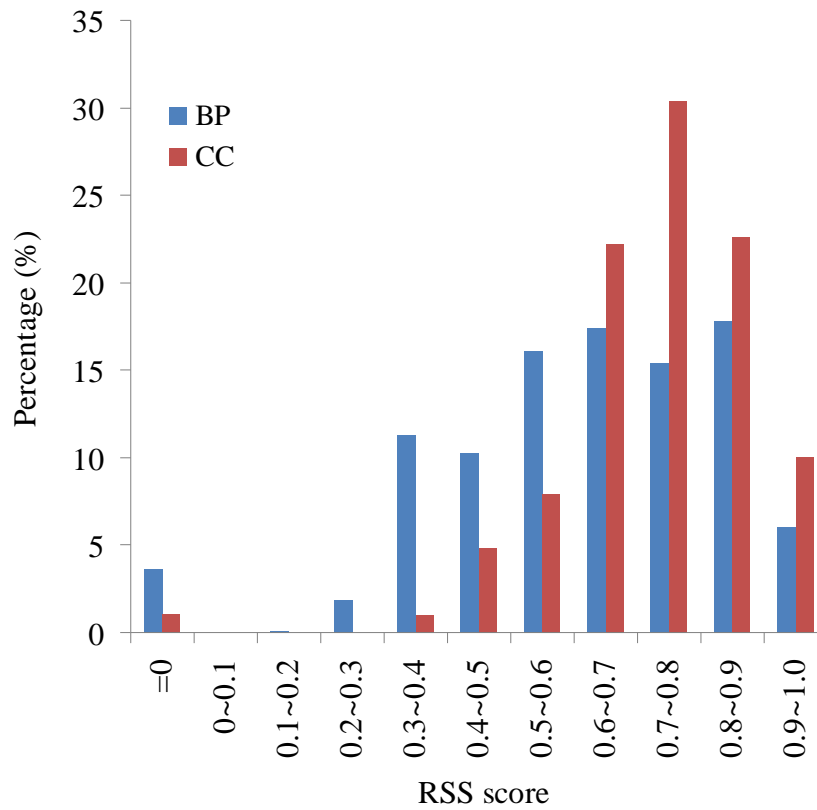


Figure S3. The distributions of the biological process (BP) and cellular component (CC) RSS scores on 84,082 protein-protein interactions selected from the IntAct database. Among 198,882 interactions recorded in IntAct, 84,082 interactions can be calculated the BP and CC RSS scores. The BP and CC RSS scores of 14,188 (16.88%) and 1,742 (2.07%) interactions, respectively, are less than 0.4.

Table S1. The list of non-redundant query structural template set (NR941)

| PDB code | | | | | | | | | | | | | | |
|----------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 12e8 | 15c8 | 1a02 | 1a0q | 1a0r | 1a2k | 1a2x | 1a4f | 1a4j | 1a4y | 1a5f | 1a6a | 1a6d | 1a6t | 1a6v |
| 1a6z | 1a7q | 1a9n | 1a9w | 1abr | 1acb | 1ad0 | 1ad9 | 1ae6 | 1agr | 1ahw | 1aik | 1ais | 1aj7 | 1akh |
| 1akj | 1all | 1an1 | 1ao7 | 1aok | 1aqq | 1aro | 1aui | 1aut | 1ava | 1avw | 1awc | 1axi | 1axt | 1ay7 |
| 1azz | 1b0n | 1b2w | 1b34 | 1b35 | 1b41 | 1b4j | 1b4u | 1b8d | 1b8m | 1baf | 1bb1 | 1bbd | 1bd2 | 1bev |
| 1bgx | 1bh9 | 1bi8 | 1bj1 | 1bln | 1blx | 1bml | 1bnd | 1bp3 | 1bql | 1bqq | 1brb | 1brc | 1buh | 1bui |
| 1bvk | 1bvn | 1bvy | 1bwu | 1bx2 | 1bz7 | 1bzx | 1c12 | 1c1e | 1c1y | 1c3a | 1c4z | 1c5b | 1c5d | 1cax |
| 1cc1 | 1cd1 | 1cd9 | 1ce1 | 1ce7 | 1cf7 | 1cfv | 1cg8 | 1cgi | 1ci6 | 1cic | 1cl7 | 1clo | 1clz | 1cmx |
| 1co7 | 1cpc | 1cr9 | 1cse | 1ct8 | 1cul | 1cxz | 1cz8 | 1d2z | 1d4m | 1d4v | 1d4x | 1d5m | 1d6r | 1d8d |
| 1dce | 1dev | 1df9 | 1dfb | 1dfj | 1dhk | 1dkf | 1dkg | 1dl7 | 1dn0 | 1doa | 1dp5 | 1dqd | 1dql | 1dqq |
| 1ds6 | 1dsf | 1dtd | 1dvv | 1dzb | 1e27 | 1e3d | 1e44 | 1e4x | 1e6e | 1e6j | 1e6v | 1e6y | 1e96 | 1e9z |
| 1eah | 1eai | 1eap | 1eaw | 1ed3 | 1eer | 1ef1 | 1efn | 1efp | 1efu | 1efx | 1egj | 1ehl | 1eja | 1ejm |
| 1ejo | 1ejx | 1em8 | 1emt | 1eo8 | 1ep2 | 1es0 | 1eth | 1etz | 1euc | 1euv | 1evt | 1ewy | 1exu | 1eys |
| 1eyx | 1ezs | 1f02 | 1f11 | 1f34 | 1f3d | 1f3m | 1f3v | 1f45 | 1f4x | 1f5q | 1f6f | 1f80 | 1f8t | 1f99 |
| 1fak | 1fbi | 1fbv | 1fc2 | 1fcd | 1fdh | 1ffv | 1fg9 | 1fgv | 1fh5 | 1fig | 1fj1 | 1fl5 | 1fle | 1flr |
| 1flt | 1fma | 1fn4 | 1fod | 1for | 1fpn | 1fpt | 1fq1 | 1fq9 | 1fqj | 1frg | 1fs0 | 1fs1 | 1fs2 | 1fss |
| 1fvc | 1fvd | 1fxk | 1fxw | 1fyh | 1fyt | 1g1x | 1g3j | 1g3n | 1g4u | 1g4y | 1g72 | 1g73 | 1gaf | 1gaq |
| 1gcq | 1gcv | 1gg2 | 1ggp | 1ghf | 1gl0 | 1gl1 | 1gl2 | 1gl4 | 1gng | 1go3 | 1got | 1gpo | 1gpq | 1gpw |
| 1gux | 1gvn | 1gzs | 1h0d | 1h0h | 1h1v | 1h2k | 1h2m | 1h2s | 1h2v | 1h3o | 1h3p | 1h4i | 1h6k | 1h9h |
| 1h9i | 1hbr | 1hcf | 1hdm | 1hds | 1he1 | 1he8 | 1hez | 1hfe | 1hh4 | 1hil | 1hl6 | 1hlu | 1hsb | 1hwg |
| 1hx1 | 1hxs | 1hyr | 1hys | 1hzh | 1i1a | 1i1q | 1i1r | 1i2m | 1i3g | 1i4o | 1i7w | 1i7z | 1i8i | 1i9c |
| 1i9j | 1iai | 1iak | 1iao | 1iar | 1ibg | 1ibr | 1igc | 1igf | 1igm | 1igt | 1ijd | 1ik9 | 1ikf | 1ikn |
| 1il1 | 1im9 | 1ind | 1iod | 1iqd | 1iqw | 1ira | 1it9 | 1itb | 1iwp | 1ixx | 1izn | 1j05 | 1j1d | 1j2j |
| 1j3k | 1j7d | 1j7v | 1j9c | 1jat | 1jbo | 1jdh | 1jeb | 1jek | 1jeq | 1jey | 1jfi | 1jfq | 1jgl | 1jgu |
| 1jhl | 1jiw | 1jju | 1jk0 | 1jk9 | 1jkg | 1jkj | 1jlt | 1jma | 1jnz | 1jnl | 1jnz | 1jps | 1jpw | 1jqj |
| 1jq1 | 1jr3 | 1jrh | 1jsi | 1jst | 1jsu | 1jtd | 1jth | 1jtp | 1jv5 | 1jy2 | 1jyo | 1jzd | 1k28 | 1k3z |
| 1k6q | 1k8d | 1k8r | 1k9o | 1ka9 | 1kac | 1kb5 | 1kc5 | 1kcr | 1kcv | 1kd8 | 1kd9 | 1kdd | 1kem | 1kf9 |
| 1kfa | 1kfu | 1kg0 | 1ki1 | 1kig | 1kil | 1kj1 | 1kjv | 1kk8 | 1kkm | 1kmc | 1kmi | 1kn1 | 1kps | 1kqf |
| 1ksg | 1kth | 1ktr | 1ktz | 1ku6 | 1kxt | 1kxv | 1kz7 | 1l0o | 1l0y | 1l1o | 1l4a | 1l4d | 1l4z | 1l7t |
| 1ld9 | 1ldt | 1le8 | 1lfd | 1li1 | 1lia | 1lk3 | 1l04 | 1lqs | 1lrw | 1lsh | 1lt3 | 1lt4 | 1ltx | 1luj |
| 1lw6 | 1m1e | 1m2o | 1m2v | 1m9d | 1mam | 1mbx | 1mcp | 1mda | 1mdu | 1mee | 1mex | 1mh2 | 1mh5 | 1mhc |
| 1mhh | 1mhp | 1mhy | 1mi5 | 1mie | 1mim | 1mio | 1mj8 | 1mk2 | 1mlc | 1mnm | 1mox | 1mpa | 1mqm | 1mqz |
| 1mr1 | 1mre | 1mty | 1mu2 | 1muj | 1mvf | 1mz8 | 1n0l | 1n0w | 1n1j | 1n2d | 1n4x | 1n54 | 1n5w | 1n62 |
| 1n6j | 1n7s | 1n8s | 1nak | 1nam | 1nbf | 1nbn | 1nbv | 1nbw | 1nby | 1nca | 1ncb | 1ncd | 1ncw | 1ndg |
| 1ndm | 1nex | 1nez | 1nf3 | 1nfi | 1ngp | 1nh2 | 1nj9 | 1nkp | 1nkz | 1nld | 1nlw | 1nmu | 1npe | 1nrj |
| 1nsn | 1nt2 | 1nu9 | 1nun | 1nvp | 1nvv | 1nw9 | 1ny7 | 1o5f | 1oak | 1oao | 1oaz | 1obl | 1oc0 | 1of5 |

Table S1. The list of non-redundant query structural template set (Continued)

| PDB code | | | | | | | | | | | | | | | |
|----------|------|------|------|------|------|------|------|------|------|------|------|-------|------|-------|------|
| lofu | lohz | loiu | lonk | lonq | loo0 | loop | lop3 | lop9 | lopg | loph | loql | lor7 | lors | lory | |
| losp | lots | louu | lowf | lows | loyv | loz7 | lp0s | lp22 | lp27 | lp2c | lp4b | lp4l | lp7k | lpdk | |
| lpx | lpg5 | lph6 | lphn | lpk1 | lpkq | lplg | lpoi | lpov | lppf | lpqz | lpsk | lpum | lpuu | lpvh | |
| lpxv | lpyt | lq0x | lq0y | lq40 | lq9w | lqav | lqbk | lqbm | lqdl | lqfu | lqgk | lqkz | lqlb | lqle | |
| lqo0 | lqo3 | lqpw | lqs0 | lqyg | lqz7 | lr0a | lr0c | lr1k | lr4p | lr5v | lr6o | lr8d | lr0e | lr0w | |
| lrfn | lrgi | lrhh | lrhi | lri8 | lrih | lrjc | lrjl | lrke | lrml | lrmf | lrrp | lr0u | lr0y | lr0z | |
| lrv6 | lrz7 | lrzf | lrzg | lrzk | lrzo | ls1q | ls4y | ls6b | ls70 | ls9v | lsb3 | lsbn | lsbs | lsbw | |
| lscj | lsdd | lseq | lsg1 | lshw | lshz | lsm3 | lsmg | lspb | lspg | lspg | lspg | lstr4 | lstf | lsv0 | lsvd |
| lsvf | lsvx | lsy6 | lsyx | lt04 | lt08 | lt0f | lt0j | lt0p | lt0q | lt2k | lt2q | lt3q | lt44 | lt4k | |
| lt61 | lt66 | lt6b | lt6g | lt83 | lt9g | lta3 | ltab | ltaf | ltaw | ltco | ltdq | lte1 | ltet | ltfx | |
| ltgs | lth1 | lti8 | ltmc | ltme | ltmq | ltnr | ltqb | lts5 | ltth | lttw | ltx6 | lty4 | ltyq | ltzg | |
| ltzh | ltzi | lu0s | lu2v | lu7f | lu7v | lua6 | luac | luad | lub4 | lub5 | lub6 | lucb | ludi | luea | |
| luex | lugh | lugq | luhl | luj3 | lujw | lujz | lukl | lukv | lul1 | luli | lum4 | lunn | lurq | lus7 | |
| lusu | luug | luuz | luvq | luw4 | luwe | luwg | luyw | luz8 | luzx | lv18 | lv29 | lv4l | lv4x | lv5i | |
| lv74 | lv7m | lv7p | lvf6 | lvg0 | lvge | lvgk | lviv | lvol | lvra | lvrq | lvrs | lv0j | lv98 | lvaw5 | |
| lwc7 | lwd | lwdk | lwmh | lwmi | lwp | lwp | lwp | lwp | lwp | lwp | lwp | lwp | lwp | lwp | |
| lxcg | lxd3 | lxd | lxew | lxg2 | lxgu | lxgy | lxhm | lxkp | lx13 | lxo2 | lxou | lxq5 | lxqs | lxr8 | |
| lxrs | lxt9 | lxtg | lxu1 | lxu2 | lxwd | lxx9 | lxxf | ly14 | ly43 | ly4z | ly56 | ly6n | ly75 | ly8r | |
| ly8x | ly96 | lya5 | lyag | lyc0 | lycs | lyd8 | lyee | lyhn | lyjd | lykh | lymh | lyph | lyqv | lyrn | |
| lytf | lytz | lyu6 | lyuh | lyuk | lyy8 | lyy9 | lz0j | lz0k | lz2c | lz3e | lz5s | lz5y | lz7k | lz7x | |
| lz92 | lza1 | lzbd | lzbe | lze3 | lzhi | lzd | lzl | lzli | lzm4 | lzmy | lzoy | lza1 | lza0 | lza4 | |
| lzt | lzud | lzun | lzvv | 2a19 | 2a1j | 2a1t | 2a5t | 2a5y | 2a6q | 2a74 | 2a9m | 2aa1 | 2aab | 2aai | |
| 2abz | 2adf | 2ae4 | 2aep | 2aka | 2aly | 2apo | 2ast | 2atc | 2atp | 2avu | 2aw2 | 2aze | 2b0u | 2b1x | |
| 2b4s | 2b59 | 2b5i | 2b5l | 2b7d | 2b7y | 2b9s | 2bbv | 2bck | 2be6 | 2beq | 2bez | 2bh1 | 2bki | 2bkk | |
| 2bku | 2bky | 2bl0 | 2blf | 2bo9 | 2bpa | 2bpt | 2brr | 2bse | 2btf | 2bto | 2c0j | 2c1m | 2c1o | 2c1p | |
| 2c51 | 2c71 | 2c9w | 2d2m | 2d9q | 2dhb | 2ey4 | 2f19 | 2f5a | 2f91 | 2f9d | 2f9j | 2fbj | 2fdb | 2fgw | |
| 2fif | 2fwo | 2h1p | 2hrp | 2iad | 2iff | 2ig2 | 2jel | 2pcp | 2prg | 2siv | 2sni | 2trc | 2vgl | 2zxx | |
| 32c2 | 3c98 | 3fhi | 3gtu | 3hfm | 3rub | 4pro | 4sgb | 7fab | 7req | 8fab | | | | | |

Table S2. Gold standard positive set

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---|
| 1a02 | P15407-P17275 | 9606 | <i>Homo sapiens</i> |
| 1a2x | P02588-P68246 | 9031 | <i>Gallus gallus</i> |
| 1a4f | P01942-P02088 | 10090 | <i>Mus musculus</i> |
| 1a4f | P01942-P02089 | 10090 | <i>Mus musculus</i> |
| 1a4f | P68871-P69905 | 9606 | <i>Homo sapiens</i> |
| 1a6a | P14434-P14483 | 10090 | <i>Mus musculus</i> |
| 1a6a | P01903-P13760 | 9606 | <i>Homo sapiens</i> |
| 1a6d | P80313-P80313 | 10090 | <i>Mus musculus</i> |
| 1a6d | P39078-P42943 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1a6d | P39079-P42943 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1a6d | P39076-P42943 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1a6d | P17987-P48643 | 9606 | <i>Homo sapiens</i> |
| 1a6d | P17987-P78371 | 9606 | <i>Homo sapiens</i> |
| 1a9n | P43332-P43332-Q9V4Q8-Q9V4Q8 | 7227 | <i>Drosophila melanogaster</i> |
| lagr | P10824-P10824-P49799-P49799 | 10116 | <i>Rattus norvegicus</i> |
| lais | P13393-P29056 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lais | P20226-Q92994 | 9606 | <i>Homo sapiens</i> |
| lais | P20226-Q00403 | 9606 | <i>Homo sapiens</i> |
| lall | Q01951-Q54714 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| lall | Q01951-Q54715 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| laro | P00573-P00806 | 10760 | <i>Enterobacteria phage T7</i> |
| loui | P62203-Q8IAM8 | 36329 | <i>Plasmodium falciparum 3D7</i> |
| loui | Q12705-Q9UU93 | 4896 | <i>Schizosaccharomyces pombe</i> |
| loui | P14747-P25296 | 4932 | <i>Saccharomyces cerevisiae</i> |
| loui | P23287-P25296 | 4932 | <i>Saccharomyces cerevisiae</i> |
| loui | P06787-P23287 | 4932 | <i>Saccharomyces cerevisiae</i> |
| loui | P06787-P14747 | 4932 | <i>Saccharomyces cerevisiae</i> |
| loui | P48451-P48456 | 7227 | <i>Drosophila melanogaster</i> |
| loui | P63098-Q08209 | 9606 | <i>Homo sapiens</i> |
| lawc | Q04688-Q9WOR7 | 7227 | <i>Drosophila melanogaster</i> |
| laxi | P01241-P10912 | 9606 | <i>Homo sapiens</i> |
| laxi | P01241-P16471 | 9606 | <i>Homo sapiens</i> |
| 1b0n | P06533-P23308 | 224308 | <i>Bacillus subtilis subsp. subtilis str. 168</i> |
| 1b8m | P20783-P23560 | 9606 | <i>Homo sapiens</i> |
| 1bh9 | P61216-Q99JX1 | 10090 | <i>Mus musculus</i> |
| 1bh9 | P49906-Q9VIP1 | 7227 | <i>Drosophila melanogaster</i> |
| 1bh9 | Q15543-Q15544 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P55273-P55273-Q00534-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P11802-P11802-P55273-P55273 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P42773-P42773-Q00534-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P11802-P11802-P42773-P42773 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P11802-P11802-P42772-P42772 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P42771-P42771-Q00534-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1bi8 | P11802-P11802-P42771-P42771 | 9606 | <i>Homo sapiens</i> |
| 1blx | P55273-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1blx | P11802-P55273 | 9606 | <i>Homo sapiens</i> |
| 1blx | P11802-P42772 | 9606 | <i>Homo sapiens</i> |
| 1blx | P42771-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1blx | P11802-P42771 | 9606 | <i>Homo sapiens</i> |
| 1blx | P42773-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1blx | P11802-P42773 | 9606 | <i>Homo sapiens</i> |
| 1bnd | P20783-P23560 | 9606 | <i>Homo sapiens</i> |
| 1bp3 | P01241-P16471 | 9606 | <i>Homo sapiens</i> |
| 1bp3 | P01241-P10912 | 9606 | <i>Homo sapiens</i> |
| 1bqq | P08253-P16035 | 9606 | <i>Homo sapiens</i> |
| 1brc | P05067-Q92876 | 9606 | <i>Homo sapiens</i> |
| 1buh | Q23249-Q8LG64 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | Q23249-Q2V419 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | Q23249-P25859 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | P25859-Q9SJJ5 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | Q23249-Q8LF80 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | Q23249-P24100 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | P24100-Q9SJJ5 | 3702 | <i>Arabidopsis thaliana</i> |
| 1buh | P00546-P20486 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1buh | P34556-Q17868 | 6239 | <i>Caenorhabditis elegans</i> |
| 1buh | P23573-Q24152 | 7227 | <i>Drosophila melanogaster</i> |
| 1buh | P23572-Q24152 | 7227 | <i>Drosophila melanogaster</i> |
| 1buh | P23573-Q9VHN1 | 7227 | <i>Drosophila melanogaster</i> |
| 1buh | P23572-Q9VHN1 | 7227 | <i>Drosophila melanogaster</i> |
| 1buh | P24941-P61024 | 9606 | <i>Homo sapiens</i> |
| 1bx2 | P14434-P14434-P14483-P14483 | 10090 | <i>Mus musculus</i> |
| 1bx2 | P01903-P01903-P13760-P13760 | 9606 | <i>Homo sapiens</i> |
| 1cly | Q61411-Q99N57 | 10090 | <i>Mus musculus</i> |
| 1cly | P04627-Q61411 | 10090 | <i>Mus musculus</i> |
| 1cly | P04049-P62834 | 9606 | <i>Homo sapiens</i> |
| 1cly | P01112-P04049 | 9606 | <i>Homo sapiens</i> |
| 1cly | P01112-P10398 | 9606 | <i>Homo sapiens</i> |
| 1cly | P01112-P15056 | 9606 | <i>Homo sapiens</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---|
| lcc1 | P0ACD8-P69741 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| lcd1 | P01887-P01887-P11609-P11609 | 10090 | <i>Mus musculus</i> |
| lcd1 | P06126-P06126-P61769-P61769 | 9606 | <i>Homo sapiens</i> |
| lcd1 | P29016-P29016-P61769-P61769 | 9606 | <i>Homo sapiens</i> |
| lcd1 | P61769-P61769-Q30201-Q30201 | 9606 | <i>Homo sapiens</i> |
| lcf7 | Q9FNY2-Q9FV71 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY2-Q9SJ49 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY2-Q9FV70 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY0-Q9FNY2 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY3-Q9FV71 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY3-Q9FV70 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY0-Q9FNY3 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q9FNY3-Q9SJ49 | 3702 | <i>Arabidopsis thaliana</i> |
| lcf7 | Q24318-Q27368 | 7227 | <i>Drosophila melanogaster</i> |
| lcf7 | O75461-Q14188 | 9606 | <i>Homo sapiens</i> |
| lcf7 | O75461-Q14186 | 9606 | <i>Homo sapiens</i> |
| lcg8 | P01942-P02089 | 10090 | <i>Mus musculus</i> |
| lcg8 | P01942-P02088 | 10090 | <i>Mus musculus</i> |
| lcg8 | P68871-P69905 | 9606 | <i>Homo sapiens</i> |
| lczx | P61586-Q16512 | 9606 | <i>Homo sapiens</i> |
| ld2z | P22812-P22812-Q05652-Q05652 | 7227 | <i>Drosophila melanogaster</i> |
| ld4v | O14763-P50591 | 9606 | <i>Homo sapiens</i> |
| ld4v | O00220-P50591 | 9606 | <i>Homo sapiens</i> |
| ld4x | Q62468-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| ld4x | P83967-Q24020 | 7227 | <i>Drosophila melanogaster</i> |
| ld8d | Q02293-Q04631 | 10116 | <i>Rattus norvegicus</i> |
| ld8d | P53610-Q04631 | 10116 | <i>Rattus norvegicus</i> |
| ld8d | P22007-P29703 | 4932 | <i>Saccharomyces cerevisiae</i> |
| ld8d | O44501-Q19752 | 6239 | <i>Caenorhabditis elegans</i> |
| ld8d | O18197-O44501 | 6239 | <i>Caenorhabditis elegans</i> |
| ld8d | P49354-P49356 | 9606 | <i>Homo sapiens</i> |
| ldev | O95405-O95405-P84022-P84022 | 9606 | <i>Homo sapiens</i> |
| ldkf | P20153-P34021 | 7227 | <i>Drosophila melanogaster</i> |
| ldkf | P20153-P49869 | 7227 | <i>Drosophila melanogaster</i> |
| ldkf | P10276-P48443 | 9606 | <i>Homo sapiens</i> |
| ldkf | P10276-P28702 | 9606 | <i>Homo sapiens</i> |
| ldkf | P48443-Q07869 | 9606 | <i>Homo sapiens</i> |
| ldoa | P60764-Q61599 | 10090 | <i>Mus musculus</i> |
| ldoa | P60764-Q99PT1 | 10090 | <i>Mus musculus</i> |
| ldoa | Q38912-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| ldoa | Q38937-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| ldoa | P19073-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| ldoa | Q00246-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| ldoa | P06780-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| ldoa | P52565-P60953 | 9606 | <i>Homo sapiens</i> |
| ldoa | P52565-P63000 | 9606 | <i>Homo sapiens</i> |
| ldoa | P08134-P52565 | 9606 | <i>Homo sapiens</i> |
| ldoa | P52565-P61586 | 9606 | <i>Homo sapiens</i> |
| ldoa | P52565-P62745 | 9606 | <i>Homo sapiens</i> |
| lds6 | P60764-Q61599 | 10090 | <i>Mus musculus</i> |
| lds6 | P60764-Q99PT1 | 10090 | <i>Mus musculus</i> |
| lds6 | Q38937-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| lds6 | Q38912-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| lds6 | Q00246-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lds6 | P06780-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lds6 | P19073-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lds6 | P52565-P63000 | 9606 | <i>Homo sapiens</i> |
| lds6 | P52565-P62745 | 9606 | <i>Homo sapiens</i> |
| lds6 | P08134-P52565 | 9606 | <i>Homo sapiens</i> |
| lds6 | P52565-P61586 | 9606 | <i>Homo sapiens</i> |
| lds6 | P52565-P60953 | 9606 | <i>Homo sapiens</i> |
| le27 | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| le3d | P0ACD8-P0ACD8-P69741-P69741 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| le3d | P0ACD8-P0ACD8-P69741-P69741 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| le96 | P15153-P19878 | 9606 | <i>Homo sapiens</i> |
| le96 | P19878-P63000 | 9606 | <i>Homo sapiens</i> |
| le96 | P19878-P60953 | 9606 | <i>Homo sapiens</i> |
| led3 | P07151-P07151-P13599-P13599 | 10116 | <i>Rattus norvegicus</i> |
| leer | P01588-P19235-P19235 | 9606 | <i>Homo sapiens</i> |
| lef1 | P26040-P26040-P46662-P46662 | 10090 | <i>Mus musculus</i> |
| lef1 | P46150-P46150-P46150-P46150 | 7227 | <i>Drosophila melanogaster</i> |
| lef1 | P46150-P46150-Q24564-Q24564 | 7227 | <i>Drosophila melanogaster</i> |
| lefp | Q9C6I6-Q9C6I6-Q9LSW8-Q9LSW8 | 3702 | <i>Arabidopsis thaliana</i> |
| lem8 | P28632-P28632-P28905-P28905 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| lem8 | P28632-P28632-P28905-P28905 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|---|----------------|---|
| lep2 | P54322-P56968 | 1358 | <i>Lactococcus lactis</i> |
| les0 | P14434-P14483 | 10090 | <i>Mus musculus</i> |
| leuc | Q0PAY2-Q9PHY1 | 192222 | <i>Campylobacter jejuni</i> subsp. <i>jejuni</i> NCTC 11168 |
| leuc | P0A836-P0AGE9 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| leuc | P53312-P53598 | 4932 | <i>Saccharomyces cerevisiae</i> |
| leuc | P0A836-P0AGE9 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| leuv | Q02724-Q12306 | 4932 | <i>Saccharomyces cerevisiae</i> |
| leuv | P63165-Q9HC62 | 9606 | <i>Homo sapiens</i> |
| levt | P05230-P05230-P22607-P22607 | 9606 | <i>Homo sapiens</i> |
| lexu | P01887-P11609 | 10090 | <i>Mus musculus</i> |
| lexu | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| lf3m | Q03497-Q03497-Q03497-Q03497 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lf3m | Q13177-Q13177-Q13177-Q13177 | 9606 | <i>Homo sapiens</i> |
| lf3v | Q12933-Q15628 | 9606 | <i>Homo sapiens</i> |
| lf99 | Q01951-Q01951-Q01951-Q54714-Q54714-Q54714 | 1148 | <i>Synechocystis</i> sp. PCC 6803 |
| lf99 | Q01951-Q01951-Q01951-Q54715-Q54715-Q54715 | 1148 | <i>Synechocystis</i> sp. PCC 6803 |
| lfbv | P68036-Q9ULV8 | 9606 | <i>Homo sapiens</i> |
| lfbv | O14933-Q9ULV8 | 9606 | <i>Homo sapiens</i> |
| lfbv | Q712K3-Q9ULV8 | 9606 | <i>Homo sapiens</i> |
| lfbv | P63279-Q9ULV8 | 9606 | <i>Homo sapiens</i> |
| lfbv | P62256-Q9ULV8 | 9606 | <i>Homo sapiens</i> |
| lfdh | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| lfdh | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| lfdh | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lfma | P30748-P30749 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| lfma | P30748-P30749 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| lfq1 | P24941-Q16667 | 9606 | <i>Homo sapiens</i> |
| lfq9 | P09038-P09038-P11362-P11362 | 9606 | <i>Homo sapiens</i> |
| lfq9 | P09038-P09038-P21802-P21802 | 9606 | <i>Homo sapiens</i> |
| lfq9 | P05230-P05230-P21802-P21802 | 9606 | <i>Homo sapiens</i> |
| lfq9 | P05230-P05230-P22607-P22607 | 9606 | <i>Homo sapiens</i> |
| lfq9 | O15520-O15520-P21802-P21802 | 9606 | <i>Homo sapiens</i> |
| lfs0 | P0A6E6-P0ABA6 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| lfs0 | P0A6E6-P0ABA6 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| lfs2 | P63208-P63208-Q13309-Q13309 | 9606 | <i>Homo sapiens</i> |
| lfxw | P68402-Q15102 | 9606 | <i>Homo sapiens</i> |
| lfxw | Q15102-Q15102 | 9606 | <i>Homo sapiens</i> |
| lfxw | P68401-Q29460 | 9913 | <i>Bos taurus</i> |
| lfyh | P01579-P01579-P15260-P15260 | 9606 | <i>Homo sapiens</i> |
| lg4y | P62161-P70604 | 10116 | <i>Rattus norvegicus</i> |
| lgcq | P27870-Q60631-Q60631 | 10090 | <i>Mus musculus</i> |
| lgcq | P15498-P62993-P62993 | 9606 | <i>Homo sapiens</i> |
| lgcq | P62993-P62993-Q9UKW4 | 9606 | <i>Homo sapiens</i> |
| lgcv | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| lgcv | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| lgcv | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lg14 | P10493-Q05793 | 10090 | <i>Mus musculus</i> |
| lgo3 | Q57840-Q57840-Q60351-Q60351 | 243232 | <i>Methanocaldococcus jannaschii</i> DSM 2661 |
| lgpw | Q7SIB9-Q7SIB9-Q7SIB9-Q7SIC0-Q7SIC0-Q7SIC0 | 300852 | <i>Thermus thermophilus</i> HB8 |
| 1h0h | P0AAJ5-P0AAJ5-P32176-P32176 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| 1h0h | P0AAJ3-P0AAJ3-P24183-P24183 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| 1h0h | P0AAJ5-P0AAJ5-P32176-P32176 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| 1h0h | P0AAJ3-P0AAJ3-P24183-P24183 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| 1h1v | Q62468-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| 1h2k | Q16665-Q9NWT6 | 9606 | <i>Homo sapiens</i> |
| 1h2m | Q16665-Q9NWT6 | 9606 | <i>Homo sapiens</i> |
| 1h2v | Q9SIU2-Q9XFD1 | 3702 | <i>Arabidopsis thaliana</i> |
| 1h2v | P52298-Q09161 | 9606 | <i>Homo sapiens</i> |
| 1h3o | O00268-O00268-Q16514-Q16514 | 9606 | <i>Homo sapiens</i> |
| 1h6k | P52298-P52298-P52298-Q09161-Q09161-Q09161 | 9606 | <i>Homo sapiens</i> |
| 1hbr | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| 1hbr | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| 1hbr | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| 1hds | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---|
| lhds | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| lhds | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lhe8 | P08646-P91634 | 7227 | <i>Drosophila melanogaster</i> |
| lhe8 | P01112-P48736 | 9606 | <i>Homo sapiens</i> |
| lhh4 | P60764-P60764-Q99PT1-Q99PT1 | 10090 | <i>Mus musculus</i> |
| lhh4 | P60764-P60764-Q61599-Q61599 | 10090 | <i>Mus musculus</i> |
| lhh4 | Q38937-Q38937-Q9SFC6-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| lhh4 | Q38912-Q38912-Q9SFC6-Q9SFC6 | 3702 | <i>Arabidopsis thaliana</i> |
| lhh4 | P19073-P19073-Q12434-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lhh4 | Q00246-Q00246-Q12434-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lhh4 | P06780-P06780-Q12434-Q12434 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lhh4 | P52565-P52565-P63000-P63000 | 9606 | <i>Homo sapiens</i> |
| lhh4 | P08134-P08134-P52565-P52565 | 9606 | <i>Homo sapiens</i> |
| lhh4 | P52565-P52565-P60953-P60953 | 9606 | <i>Homo sapiens</i> |
| lhh4 | P52565-P52565-P61586-P61586 | 9606 | <i>Homo sapiens</i> |
| lhh4 | P52565-P52565-P62745-P62745 | 9606 | <i>Homo sapiens</i> |
| lhl6 | P49029-P49029-Q21832-Q21832 | 6239 | <i>Caenorhabditis elegans</i> |
| lhl6 | P49028-P49028-Q9V535-Q9V535 | 7227 | <i>Drosophila melanogaster</i> |
| lhl6 | Q96A72-Q96A72-Q9Y5S9-Q9Y5S9 | 9606 | <i>Homo sapiens</i> |
| lhl6 | P61326-P61326-Q9Y5S9-Q9Y5S9 | 9606 | <i>Homo sapiens</i> |
| lhl6 | P35080-P63261 | 9606 | <i>Homo sapiens</i> |
| lhsb | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| lilq | Q06128-Q06129 | 273057 | <i>Sulfolobus solfataricus P2</i> |
| lilq | P00899-P00937 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lilq | P00898-P00905 | 99287 | <i>Salmonella enterica subsp. enterica serovar Typhimurium str. LT2</i> |
| li4o | P55210-P55210-P98170-P98170 | 9606 | <i>Homo sapiens</i> |
| li4o | P55210-P55210-Q13490-Q13490 | 9606 | <i>Homo sapiens</i> |
| li4o | P42574-P42574-P98170-P98170 | 9606 | <i>Homo sapiens</i> |
| li4o | P42574-P42574-Q13490-Q13490 | 9606 | <i>Homo sapiens</i> |
| liak | P14434-P14483 | 10090 | <i>Mus musculus</i> |
| liao | P14434-P14483 | 10090 | <i>Mus musculus</i> |
| liar | P05112-P24394 | 9606 | <i>Homo sapiens</i> |
| libr | P32835-P32835-Q06142-Q06142 | 4932 | <i>Saccharomyces cerevisiae</i> |
| libr | P62826-P62826-Q14974-Q14974 | 9606 | <i>Homo sapiens</i> |
| lik9 | P49917-Q13426-Q13426 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-P25963-Q04206 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q04206-Q04206 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q04206-Q04864 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-P25963-Q00653 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-P25963-Q04864 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-P25963-Q01201 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q00653-Q00653 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q00653-Q04864 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q00653-Q01201 | 9606 | <i>Homo sapiens</i> |
| likn | P25963-Q04864-Q04864 | 9606 | <i>Homo sapiens</i> |
| likn | Q04206-Q04206-Q15653 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-Q04206-Q15653 | 9606 | <i>Homo sapiens</i> |
| likn | P19838-Q00653-Q15653 | 9606 | <i>Homo sapiens</i> |
| likn | Q04206-Q04864-Q15653 | 9606 | <i>Homo sapiens</i> |
| likn | Q00653-Q00653-Q15653 | 9606 | <i>Homo sapiens</i> |
| lira | P14778-P18510 | 9606 | <i>Homo sapiens</i> |
| litb | P10749-P13504 | 10090 | <i>Mus musculus</i> |
| litb | P01584-P14778 | 9606 | <i>Homo sapiens</i> |
| lj2j | P84077-Q9UJY5 | 9606 | <i>Homo sapiens</i> |
| lj7d | O97241-Q8I3J4 | 36329 | <i>Plasmodium falciparum 3D7</i> |
| lj7d | Q94A97-Q9CAB6 | 3702 | <i>Arabidopsis thaliana</i> |
| lj7d | P52490-P53152 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lj7d | P53152-Q02159 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lj7d | O45495-Q95XX0 | 6239 | <i>Caenorhabditis elegans</i> |
| lj7d | P61088-Q13404 | 9606 | <i>Homo sapiens</i> |
| lj7d | P61088-Q15819 | 9606 | <i>Homo sapiens</i> |
| lj7v | P22301-Q13651 | 9606 | <i>Homo sapiens</i> |
| lj9c | P08709-P08709-P13726 | 9606 | <i>Homo sapiens</i> |
| ljat | O97241-Q8I3J4 | 36329 | <i>Plasmodium falciparum 3D7</i> |
| ljat | Q94A97-Q9CAB6 | 3702 | <i>Arabidopsis thaliana</i> |
| ljat | P52490-P53152 | 4932 | <i>Saccharomyces cerevisiae</i> |
| ljat | O45495-Q95XX0 | 6239 | <i>Caenorhabditis elegans</i> |
| ljat | P61088-Q13404 | 9606 | <i>Homo sapiens</i> |
| ljat | P61088-Q15819 | 9606 | <i>Homo sapiens</i> |
| ljbo | Q01951-Q54714 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| ljbo | Q01951-Q54715 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| ljeb | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| ljeb | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| ljeb | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| ljeq | P23475-P27641 | 10090 | <i>Mus musculus</i> |
| ljeq | Q6AZ64-Q6P7P8 | 10116 | <i>Rattus norvegicus</i> |
| ljeq | P12956-P13010 | 9606 | <i>Homo sapiens</i> |
| ljey | P23475-P27641 | 10090 | <i>Mus musculus</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|---|----------------|---|
| 1jey | Q6AZ64-Q6P7P8 | 10116 | <i>Rattus norvegicus</i> |
| 1jey | P12956-P13010 | 9606 | <i>Homo sapiens</i> |
| 1jk0 | P09938-P49723 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1jk0 | P42170-P42170 | 6239 | <i>Caenorhabditis elegans</i> |
| 1jkg | Q9U757-Q9XVS8 | 6239 | <i>Caenorhabditis elegans</i> |
| 1jkg | Q9U1H9-Q9V3H8 | 7227 | <i>Drosophila melanogaster</i> |
| 1jkg | Q9UBU9-Q9UKK6 | 9606 | <i>Homo sapiens</i> |
| 1jkg | Q9H4D5-Q9NPJ8 | 9606 | <i>Homo sapiens</i> |
| 1jkg | Q9H4D5-Q9UKK6 | 9606 | <i>Homo sapiens</i> |
| 1jqj | P0A988-P0A988-P28630-P28630 | 316407 | <i>Escherichia coli str. K-12</i> substr. W3110 |
| 1jqj | P0A988-P0A988-P28630-P28630 | 511145 | <i>Escherichia coli str. K-12</i> substr. MG1655 |
| 1jq1 | P0A988-P28630 | 316407 | <i>Escherichia coli str. K-12</i> substr. W3110 |
| 1jq1 | P0A988-P28630 | 511145 | <i>Escherichia coli str. K-12</i> substr. MG1655 |
| 1jsu | P24941-P46527-P78396 | 9606 | <i>Homo sapiens</i> |
| 1jsu | P20248-P24941-P46527 | 9606 | <i>Homo sapiens</i> |
| 1jth | O09044-O09044-P70452 | 10090 | <i>Mus musculus</i> |
| 1jth | P32851-P32851-P60881-P60881 | 10116 | <i>Rattus norvegicus</i> |
| 1jth | O70377-O70377-Q08850-Q08850 | 10116 | <i>Rattus norvegicus</i> |
| 1jth | Q24547-Q24547-Q9VH76-Q9VH76 | 7227 | <i>Drosophila melanogaster</i> |
| 1jth | P36975-P36975-Q24547-Q24547 | 7227 | <i>Drosophila melanogaster</i> |
| 1jth | P60880-P60880-Q16623-Q16623 | 9606 | <i>Homo sapiens</i> |
| 1jth | O75558-O75558-P60880-P60880 | 9606 | <i>Homo sapiens</i> |
| 1jth | O00161-O00161-O75558-O75558 | 9606 | <i>Homo sapiens</i> |
| 1k28 | P16009-P17172 | 10665 | <i>Enterobacteria phage T4</i> |
| 1k3z | Q04206-Q04206-Q15653 | 9606 | <i>Homo sapiens</i> |
| 1k3z | P25963-Q04206-Q04206 | 9606 | <i>Homo sapiens</i> |
| 1k3z | Q04864-Q04864-Q15653 | 9606 | <i>Homo sapiens</i> |
| 1k3z | Q00653-Q00653-Q15653 | 9606 | <i>Homo sapiens</i> |
| 1k3z | P25963-Q00653-Q00653 | 9606 | <i>Homo sapiens</i> |
| 1k3z | O00221-Q00653-Q00653 | 9606 | <i>Homo sapiens</i> |
| 1k3z | P25963-Q04864-Q04864 | 9606 | <i>Homo sapiens</i> |
| 1k3z | O00221-Q01201-Q01201 | 9606 | <i>Homo sapiens</i> |
| 1k3z | O00221-Q04864-Q04864 | 9606 | <i>Homo sapiens</i> |
| 1k8d | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 1ka9 | Q7SIB9-Q7SIC0 | 300852 | <i>Thermus thermophilus HB8</i> |
| 1kfu | Q07009-Q64537 | 10116 | <i>Rattus norvegicus</i> |
| 1kfu | P04632-P17655 | 9606 | <i>Homo sapiens</i> |
| 1kil | P60953-P60953-Q15811-Q15811 | 9606 | <i>Homo sapiens</i> |
| 1kil | P62745-P62745-Q92888-Q92888 | 9606 | <i>Homo sapiens</i> |
| 1kil | P61586-P61586-Q9NZN5-Q9NZN5 | 9606 | <i>Homo sapiens</i> |
| 1kil | O15085-O15085-P61586-P61586 | 9606 | <i>Homo sapiens</i> |
| 1kil | P62745-P62745-Q8N5V2-Q8N5V2 | 9606 | <i>Homo sapiens</i> |
| 1kil | P32851-P60881-P60881-P63041-P63045 | 10116 | <i>Rattus norvegicus</i> |
| 1kju | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 1kmc | P55210-P55210-P98170-P98170 | 9606 | <i>Homo sapiens</i> |
| 1kmc | P42574-P42574-P98170-P98170 | 9606 | <i>Homo sapiens</i> |
| 1kmc | P55210-P55210-Q13490-Q13490 | 9606 | <i>Homo sapiens</i> |
| 1kmc | P42574-P42574-Q13490-Q13490 | 9606 | <i>Homo sapiens</i> |
| 1kn1 | Q01951-Q54714 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| 1kn1 | Q01951-Q54715 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| 1ksg | O45379-Q18268 | 6239 | <i>Caenorhabditis elegans</i> |
| 1ksg | O43924-P36404 | 9606 | <i>Homo sapiens</i> |
| 1ksg | O43924-P36405 | 9606 | <i>Homo sapiens</i> |
| 1ksg | O43924-Q9NXU5 | 9606 | <i>Homo sapiens</i> |
| 1ktz | P10600-P37173 | 9606 | <i>Homo sapiens</i> |
| 111o | P15927-P15927-P27694-P27694-P35244-P35244 | 9606 | <i>Homo sapiens</i> |
| 114a | P32851-P60881-P60881-P63045 | 10116 | <i>Rattus norvegicus</i> |
| 11d9 | P07151-P07151-P13599-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 11fd | P08556-P08556-Q61193-Q61193 | 10090 | <i>Mus musculus</i> |
| 11fd | Q12967-Q12967-Q99578-Q99578 | 9606 | <i>Homo sapiens</i> |
| 11fd | Q99578-Q99578-Q9NZL6-Q9NZL6 | 9606 | <i>Homo sapiens</i> |
| 11fd | Q12967-Q12967-Q92963-Q92963 | 9606 | <i>Homo sapiens</i> |
| 11fd | P01112-P01112-Q12967-Q12967 | 9606 | <i>Homo sapiens</i> |
| 11fd | P01112-P01112-Q9NZL6-Q9NZL6 | 9606 | <i>Homo sapiens</i> |
| 11fd | Q92963-Q92963-Q9NZL6-Q9NZL6 | 9606 | <i>Homo sapiens</i> |
| 11uj | P14923-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| 11uj | P35222-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| 1m1e | P14923-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| 1m1e | P35222-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| 1m2v | P15303-P40482 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1m2v | P15303-P53953 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1m2v | P15303-P38810 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1m2v | P53992-Q15436 | 9606 | <i>Homo sapiens</i> |
| 1m2v | P53992-Q15437 | 9606 | <i>Homo sapiens</i> |
| 1m2v | O94855-Q15437 | 9606 | <i>Homo sapiens</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|--|----------------|--|
| 1m2v | O95487-Q15436 | 9606 | <i>Homo sapiens</i> |
| 1mbx | P0A8Q6-P0A8Q6-P0ABH9-P0ABH9 | 316407 | <i>Escherichia coli str. K-12 substr. W3110</i> |
| 1mbx | P0A8Q6-P0A8Q6-P0ABH9-P0ABH9 | 511145 | <i>Escherichia coli str. K-12 substr. MG1655</i> |
| 1mdu | Q62468-Q62468-Q9QZ83-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| 1mhc | P07151-P07151-P13599-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 1mk2 | O95405-P84022 | 9606 | <i>Homo sapiens</i> |
| 1mox | P00533-P00533-P01135-P01135 | 9606 | <i>Homo sapiens</i> |
| 1mq5 | P22213-Q01590 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1mr1 | P12755-P12755-Q13485-Q13485 | 9606 | <i>Homo sapiens</i> |
| 1mr1 | P12755-P12755-P84022-P84022 | 9606 | <i>Homo sapiens</i> |
| 1n0w | P51587-Q06609 | 9606 | <i>Homo sapiens</i> |
| 1nlj | P13434-Q02516 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1nlj | O17072-O17286 | 6239 | <i>Caenorhabditis elegans</i> |
| 1nlj | P25208-Q13952 | 9606 | <i>Homo sapiens</i> |
| 1n2d | P19524-P53141-P53141 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1n2d | P06787-P06787-P19524 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1n54 | Q9SIU2-Q9XFD1 | 3702 | <i>Arabidopsis thaliana</i> |
| 1n54 | P52298-Q09161 | 9606 | <i>Homo sapiens</i> |
| 1n7s | P32851-P60881-P60881-P63045 | 10116 | <i>Rattus norvegicus</i> |
| 1nbn | P0ABA6-P0ABB0-P0ABB0-P0ABB0-P0ABB4 -P0ABB4-P0ABB4 | 316407 | <i>Escherichia coli str. K-12 substr. W3110</i> |
| 1nbn | P0ABA6-P0ABB0-P0ABB0-P0ABB0-P0ABB4 -P0ABB4-P0ABB4 | 511145 | <i>Escherichia coli str. K-12 substr. MG1655</i> |
| 1nex | P07834-P07834-P52286-P52286 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1nf3 | P60766-P60766-Q9JK83-Q9JK83 | 10090 | <i>Mus musculus</i> |
| 1nf3 | Q05062-Q05062-Q9NAN2-Q9NAN2 | 6239 | <i>Caenorhabditis elegans</i> |
| 1nf3 | O97111-O97111-P40792-P40792 | 7227 | <i>Drosophila melanogaster</i> |
| 1nf3 | P60953-P60953-Q9BYG5-Q9BYG5 | 9606 | <i>Homo sapiens</i> |
| 1nf3 | P60953-P60953-Q9NPB6-Q9NPB6 | 9606 | <i>Homo sapiens</i> |
| 1nf3 | P63000-P63000-Q9BYG5-Q9BYG5 | 9606 | <i>Homo sapiens</i> |
| 1nf3 | P60953-P60953-Q9BYG4-Q9BYG4 | 9606 | <i>Homo sapiens</i> |
| 1nf3 | P63000-P63000-Q9NPB6-Q9NPB6 | 9606 | <i>Homo sapiens</i> |
| 1nf3 | P63000-P63000-Q9BYG4-Q9BYG4 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P25799-P25799-P25799-P25799-Q04207 -Q04207 | 10090 | <i>Mus musculus</i> |
| 1nfi | P25799-P25799-P25799-P25799-P25799 -P25799 | 10090 | <i>Mus musculus</i> |
| 1nfi | P19838-P19838-P25963-P25963-Q04206 -Q04206 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P25963-P25963-Q04206-Q04206-Q04206 -Q04206 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-P25963-P25963-Q04864 -Q04864 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-P25963-P25963-Q00653 -Q00653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P25963-P25963-Q00653-Q00653-Q04864 -Q04864 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P25963-P25963-Q00653-Q00653-Q00653 -Q00653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-Q04206-Q04206-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | Q04206-Q04206-Q04206-Q04206-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-P25963-P25963-Q01201 -Q01201 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-P19838-P19838-Q04864 -Q04864 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-Q00653-Q00653-Q04864 -Q04864 | 9606 | <i>Homo sapiens</i> |
| 1nfi | Q00653-Q00653-Q00653-Q00653-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-P19838-P19838-Q00653 -Q00653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | Q00653-Q00653-Q04864-Q04864-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-Q00653-Q00653-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P25963-P25963-Q00653-Q00653-Q01201 -Q01201 | 9606 | <i>Homo sapiens</i> |
| 1nfi | P19838-P19838-Q04864-Q04864-Q15653 -Q15653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-Q00653-Q00653-Q00653 -Q00653 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-P19838-P19838-Q01201 -Q01201 | 9606 | <i>Homo sapiens</i> |
| 1nfi | O00221-O00221-Q00653-Q00653-Q01201 -Q01201 | 9606 | <i>Homo sapiens</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|---|----------------|---|
| lnfi | P19838-P19838-Q00653-Q00653-Q04864-Q04864 | 9606 | <i>Homo sapiens</i> |
| lnfi | P19838-P19838-Q04206-Q04206-Q04206-Q04206 | 9606 | <i>Homo sapiens</i> |
| lnfi | P19838-P19838-Q00653-Q00653-Q00653-Q00653 | 9606 | <i>Homo sapiens</i> |
| lnkp | P01106-P01106-P61244-P61244 | 9606 | <i>Homo sapiens</i> |
| lnkp | P04198-P04198-P61244-P61244 | 9606 | <i>Homo sapiens</i> |
| lnrj | P32916-P36057 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lnr2 | O28191-O28192 | 224325 | <i>Archaeoglobus fulgidus</i> DSM 4304 |
| lnun | P91672-Q09147 | 7227 | <i>Drosophila melanogaster</i> |
| lnun | O15520-P21802 | 9606 | <i>Homo sapiens</i> |
| lnun | P09038-P21802 | 9606 | <i>Homo sapiens</i> |
| lnun | P05230-P21802 | 9606 | <i>Homo sapiens</i> |
| lnun | P09038-P11362 | 9606 | <i>Homo sapiens</i> |
| lnun | P05230-P22607 | 9606 | <i>Homo sapiens</i> |
| lnvp | P20226-P52655-P52655-P52657 | 9606 | <i>Homo sapiens</i> |
| lnvp | P52655-P52655-P52657-P62380 | 9606 | <i>Homo sapiens</i> |
| lnvv | P01112-P01112-Q07889 | 9606 | <i>Homo sapiens</i> |
| lnw9 | P55211-P98170 | 9606 | <i>Homo sapiens</i> |
| lnw9 | P55211-Q96CA5 | 9606 | <i>Homo sapiens</i> |
| lnw9 | P55211-Q13490 | 9606 | <i>Homo sapiens</i> |
| lnw9 | P55210-P98170 | 9606 | <i>Homo sapiens</i> |
| lnw9 | Q13490-Q14790 | 9606 | <i>Homo sapiens</i> |
| lnw9 | P55210-Q13490 | 9606 | <i>Homo sapiens</i> |
| loc0 | P04004-P05121 | 9606 | <i>Homo sapiens</i> |
| loiu | P97377-P97377-Q61456-Q61456 | 10090 | <i>Mus musculus</i> |
| loiu | P51943-P51943-P97377-P97377 | 10090 | <i>Mus musculus</i> |
| loiu | P11440-P11440-Q61456-Q61456 | 10090 | <i>Mus musculus</i> |
| loiu | P11440-P11440-P51943-P51943 | 10090 | <i>Mus musculus</i> |
| loiu | Q63699-Q63699-Q6AY13-Q6AY13 | 10116 | <i>Rattus norvegicus</i> |
| loiu | Q63699-Q63699-Q6GX89-Q6GX89 | 10116 | <i>Rattus norvegicus</i> |
| loiu | P39951-P39951-Q6AY13-Q6AY13 | 10116 | <i>Rattus norvegicus</i> |
| loiu | P39951-P39951-Q6GX89-Q6GX89 | 10116 | <i>Rattus norvegicus</i> |
| loiu | P04551-P04551-P10815-P10815 | 4896 | <i>Schizosaccharomyces pombe</i> |
| loiu | P04551-P04551-P36630-P36630 | 4896 | <i>Schizosaccharomyces pombe</i> |
| loiu | P00546-P00546-P24869-P24869 | 4932 | <i>Saccharomyces cerevisiae</i> |
| loiu | P20439-P20439-P23572-P23572 | 7227 | <i>Drosophila melanogaster</i> |
| loiu | P23572-P23572-Q9I7I0-Q9I7I0 | 7227 | <i>Drosophila melanogaster</i> |
| loiu | P14785-P14785-P23573-P23573 | 7227 | <i>Drosophila melanogaster</i> |
| loiu | P20248-P20248-P24941-P24941 | 9606 | <i>Homo sapiens</i> |
| loiu | P24941-P24941-P78396-P78396 | 9606 | <i>Homo sapiens</i> |
| loiu | P06493-P06493-P20248-P20248 | 9606 | <i>Homo sapiens</i> |
| lonq | P01887-P01887-P11609-P11609 | 10090 | <i>Mus musculus</i> |
| lonq | P06126-P06126-P61769-P61769 | 9606 | <i>Homo sapiens</i> |
| lonq | P29016-P29016-P61769-P61769 | 9606 | <i>Homo sapiens</i> |
| loo0 | P49029-Q21832 | 6239 | <i>Caenorhabditis elegans</i> |
| loo0 | P49028-Q9Y535 | 7227 | <i>Drosophila melanogaster</i> |
| loo0 | P61326-Q9Y5S9 | 9606 | <i>Homo sapiens</i> |
| loo0 | Q96A72-Q9Y5S9 | 9606 | <i>Homo sapiens</i> |
| lory | O67803-O67806 | 224324 | <i>Aquifex aeolicus</i> VF5 |
| louu | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| louu | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| louu | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lowf | P0A6X7-P0A6Y1 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| lowf | P0A6X7-P0A6Y1 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| lp22 | O44382-O77430 | 7227 | <i>Drosophila melanogaster</i> |
| lp22 | P63208-Q9Y297 | 9606 | <i>Homo sapiens</i> |
| lp22 | P63208-Q9UKB1 | 9606 | <i>Homo sapiens</i> |
| lpg5 | P74766-Q55338 | 330779 | <i>Sulfolobus acidocaldarius</i> DSM 639 |
| lphn | Q01951-Q54714 | 1148 | <i>Synechocystis</i> sp. PCC 6803 |
| lphn | Q01951-Q54715 | 1148 | <i>Synechocystis</i> sp. PCC 6803 |
| lpk1 | Q8IXK0-Q8IXK0-Q96GD3-Q96GD3 | 9606 | <i>Homo sapiens</i> |
| lpvh | P15018-P15018-P40189-P40189 | 9606 | <i>Homo sapiens</i> |
| lqbk | P32835-P38217 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lqbk | P32836-P38217 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lqbk | P62826-Q92973 | 9606 | <i>Homo sapiens</i> |
| lqdl | Q06128-Q06129 | 273057 | <i>Sulfolobus solfataricus</i> P2 |
| lqdl | P00899-P00937 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lqdl | P00898-P00905 | 99287 | <i>Salmonella enterica</i> subsp. enterica serovar Typhimurium str. LT2 |
| lqpw | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| lqpw | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| lqpw | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lqs0 | Q5SLR3-Q5SLR4 | 300852 | <i>Thermus thermophilus</i> HB8 |
| lqs0 | P16387-P32473 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lqs0 | Q4A1S8-Q93619 | 6239 | <i>Caenorhabditis elegans</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---|
| lqs0 | O44451-O45924 | 6239 | <i>Caenorhabditis elegans</i> |
| lqs0 | P12694-P21953 | 9606 | <i>Homo sapiens</i> |
| lrlk | P20153-P34021 | 7227 | <i>Drosophila melanogaster</i> |
| lrlk | P20153-P49869 | 7227 | <i>Drosophila melanogaster</i> |
| lrlk | P10276-P28702 | 9606 | <i>Homo sapiens</i> |
| lrlk | P10276-P48443 | 9606 | <i>Homo sapiens</i> |
| lrlk | P03372-Q96R11 | 9606 | <i>Homo sapiens</i> |
| lr5v | P14434-P14434-P14483-P14483 | 10090 | <i>Mus musculus</i> |
| lr6o | P0A8Q6-P0A8Q6-P0ABH9-P0ABH9 | 316407 | <i>Escherichia coli str. K-12</i> substr. W3110 |
| lr6o | P0A8Q6-P0A8Q6-P0ABH9-P0ABH9 | 511145 | <i>Escherichia coli str. K-12</i> substr. MG1655 |
| lre0 | P84077-Q99418 | 9606 | <i>Homo sapiens</i> |
| lrgi | Q62468-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| lrgi | P83967-Q24020 | 7227 | <i>Drosophila melanogaster</i> |
| lrrp | P41916-P41916-Q9LMK7-Q9LMK7 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | Q8H156-Q8H156-Q9LMK7-Q9LMK7 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | P41916-P41916-Q8RWG8-Q8RWG8 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | Q8H156-Q8H156-Q8RWG8-Q8RWG8 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | P41917-P41917-Q9LMK7-Q9LMK7 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | P41917-P41917-Q8RWG8-Q8RWG8 | 3702 | <i>Arabidopsis thaliana</i> |
| lrrp | P32835-P32835-P41920-P41920 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lrrp | O17915-O17915-Q86G90-Q86G90 | 6239 | <i>Caenorhabditis elegans</i> |
| lrrp | O17915-O17915-Q21021-Q21021 | 6239 | <i>Caenorhabditis elegans</i> |
| lrrp | P43487-P43487-P62826-P62826 | 9606 | <i>Homo sapiens</i> |
| ls1q | P62988-P62988-Q99816-Q99816 | 9606 | <i>Homo sapiens</i> |
| ls70 | P48462-Q86R99 | 7227 | <i>Drosophila melanogaster</i> |
| ls70 | P48462-Q8SY34 | 7227 | <i>Drosophila melanogaster</i> |
| ls70 | O14974-P62140 | 9606 | <i>Homo sapiens</i> |
| ls9v | P14434-P14434-P14483-P14483 | 10090 | <i>Mus musculus</i> |
| lshw | O08543-P54763 | 10090 | <i>Mus musculus</i> |
| lshw | O08543-Q60629 | 10090 | <i>Mus musculus</i> |
| lshz | Q14344-Q14344-Q92888-Q92888 | 9606 | <i>Homo sapiens</i> |
| lspg | P01942-P02088 | 10090 | <i>Mus musculus</i> |
| lspg | P01942-P02089 | 10090 | <i>Mus musculus</i> |
| lspg | P68871-P69905 | 9606 | <i>Homo sapiens</i> |
| lt08 | P14923-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| lt08 | P35222-Q9NSA3 | 9606 | <i>Homo sapiens</i> |
| lt0p | P20701-P32942 | 9606 | <i>Homo sapiens</i> |
| lt44 | Q62468-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| lt44 | P83967-Q24020 | 7227 | <i>Drosophila melanogaster</i> |
| ltaf | P49847-Q27272 | 7227 | <i>Drosophila melanogaster</i> |
| ltaw | P05067-Q92876 | 9606 | <i>Homo sapiens</i> |
| ltdq | P07897-Q05546 | 10116 | <i>Rattus norvegicus</i> |
| lth5 | Q12059-Q12059-Q99344-Q99344 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lty4 | O61667-O61667-P41958-P41958 | 6239 | <i>Caenorhabditis elegans</i> |
| lu0s | Q56310-Q56312 | 243274 | <i>Thermotoga maritima MSB8</i> |
| luea | P08253-P08253-P16035-P16035 | 9606 | <i>Homo sapiens</i> |
| luhl | P20153-P34021 | 7227 | <i>Drosophila melanogaster</i> |
| luhl | P20153-P49869 | 7227 | <i>Drosophila melanogaster</i> |
| luhl | P10276-P48443 | 9606 | <i>Homo sapiens</i> |
| luhl | P10276-P28702 | 9606 | <i>Homo sapiens</i> |
| luhl | P48443-Q07869 | 9606 | <i>Homo sapiens</i> |
| lukv | P09527-P37727 | 10116 | <i>Rattus norvegicus</i> |
| lukv | P01123-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32939-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P38555-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P07560-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P36017-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P39958-Q99260 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P39958-P51996 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P01123-P32864 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P36019-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P36018-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P38146-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P39958-P48559 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P38555 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P32939 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P07560-P32864 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P36017 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-Q99260 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P36019 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P36018 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lukv | P32864-P38146 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lus7 | P08238-Q16543 | 9606 | <i>Homo sapiens</i> |
| lus7 | P07900-Q16543 | 9606 | <i>Homo sapiens</i> |
| lusu | P02829-Q12449 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lusu | P15108-Q12449 | 4932 | <i>Saccharomyces cerevisiae</i> |
| luw4 | Q9BZ17-Q9BZ17-Q9HAU5-Q9HAU5 | 9606 | <i>Homo sapiens</i> |
| lv18 | P25054-P35222 | 9606 | <i>Homo sapiens</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|--|----------------|--|
| lv4x | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| lv4x | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| lv4x | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| lvg0 | P09527-P37727 | 10116 | <i>Rattus norvegicus</i> |
| lvg0 | P01123-P32864 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-Q99260 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P39958-Q99260 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P01123-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P07560-P32864 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P32939 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P07560-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32939-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P38555 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P38555-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P39958-P51996 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P36017 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P36017-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P36019 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P36018 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P36019-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P32864-P38146 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P36018-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvg0 | P38146-P39958 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lvgl | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| lvol | P20226-Q00403 | 9606 | <i>Homo sapiens</i> |
| lv0j | P0ABA6-P0ABB0-P0ABBO-P0ABBO-P0ABB4 -P0ABB4-P0ABB4 | 316407 | <i>Escherichia coli str. K-12 substr. W3110</i> |
| lv0j | P0ABA6-P0ABB0-P0ABBO-P0ABBO-P0ABB4 -P0ABB4-P0ABB4 | 511145 | <i>Escherichia coli str. K-12 substr. MG1655</i> |
| lw98 | P97377-Q61457 | 10090 | <i>Mus musculus</i> |
| lw98 | P97377-Q9Z238 | 10090 | <i>Mus musculus</i> |
| lw98 | P11440-Q61457 | 10090 | <i>Mus musculus</i> |
| lw98 | P97377-Q61456 | 10090 | <i>Mus musculus</i> |
| lw98 | P97377-Q810T2 | 10090 | <i>Mus musculus</i> |
| lw98 | P11440-Q61456 | 10090 | <i>Mus musculus</i> |
| lw98 | P11440-P24860 | 10090 | <i>Mus musculus</i> |
| lw98 | P51943-P97377 | 10090 | <i>Mus musculus</i> |
| lw98 | P11440-P51943 | 10090 | <i>Mus musculus</i> |
| lw98 | P11440-P30276 | 10090 | <i>Mus musculus</i> |
| lw98 | P39949-Q63699 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | Q63699-Q6AY13 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | P39951-Q6AY13 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | P30277-P39951 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | Q63699-Q6GX89 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | P39951-Q6GX89 | 10116 | <i>Rattus norvegicus</i> |
| lw98 | P24100-Q38819 | 3702 | <i>Arabidopsis thaliana</i> |
| lw98 | Q147G5-Q8LF80 | 3702 | <i>Arabidopsis thaliana</i> |
| lw98 | P24100-P30183 | 3702 | <i>Arabidopsis thaliana</i> |
| lw98 | P25859-P30183 | 3702 | <i>Arabidopsis thaliana</i> |
| lw98 | Q39068-Q8LF80 | 3702 | <i>Arabidopsis thaliana</i> |
| lw98 | P04551-P10815 | 4896 | <i>Schizosaccharomyces pombe</i> |
| lw98 | P04551-P36630 | 4896 | <i>Schizosaccharomyces pombe</i> |
| lw98 | P00546-P30283 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lw98 | P00546-P24869 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lw98 | P23572-P54733 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P23573-P54733 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P48609-P54733 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P14785-P23573 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P14785-P23572 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P20439-P23572 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P23572-Q917I0 | 7227 | <i>Drosophila melanogaster</i> |
| lw98 | P24864-P24941 | 9606 | <i>Homo sapiens</i> |
| lw98 | O96020-Q00526 | 9606 | <i>Homo sapiens</i> |
| lw98 | O96020-P24941 | 9606 | <i>Homo sapiens</i> |
| lw98 | P24941-P78396 | 9606 | <i>Homo sapiens</i> |
| lw98 | P06493-P78396 | 9606 | <i>Homo sapiens</i> |
| lw98 | P06493-P14635 | 9606 | <i>Homo sapiens</i> |
| lw98 | P20248-P24941 | 9606 | <i>Homo sapiens</i> |
| lw98 | O95067-P24941 | 9606 | <i>Homo sapiens</i> |
| lw98 | P06493-P20248 | 9606 | <i>Homo sapiens</i> |
| lw98 | O95067-P06493 | 9606 | <i>Homo sapiens</i> |
| lwa5 | P32835-P33307-Q02821 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lwa5 | P32836-P33307-Q02821 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lwmh | Q05513-Q9BYG5 | 9606 | <i>Homo sapiens</i> |
| lwmh | Q05513-Q9BYG4 | 9606 | <i>Homo sapiens</i> |
| lwmh | Q05513-Q9NPB6 | 9606 | <i>Homo sapiens</i> |
| lwmh | P41743-Q9BYG5 | 9606 | <i>Homo sapiens</i> |
| lwmh | P41743-Q9BYG4 | 9606 | <i>Homo sapiens</i> |
| lwmh | P41743-Q9NPB6 | 9606 | <i>Homo sapiens</i> |
| lwmi | O73966-O73966-O73967-O73967 | 70601 | <i>Pyrococcus horikoshii OT3</i> |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---|
| lwpX | P00729-P14306 | 4932 | <i>Saccharomyces cerevisiae</i> |
| lwq1 | P01112-P20936 | 9606 | <i>Homo sapiens</i> |
| lwq1 | Q53122-Q53123 | 101510 | <i>Rhodococcus jostii</i> RHA1 |
| 1x79 | Q15276-Q15276-Q9UJY4 | 9606 | <i>Homo sapiens</i> |
| 1x79 | Q15276-Q15276-Q9UJY5 | 9606 | <i>Homo sapiens</i> |
| 1x79 | Q15276-Q15276-Q9NZ52 | 9606 | <i>Homo sapiens</i> |
| 1xb2 | P0A6N1-P0A6P1 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| 1xb2 | P0A6N1-P0A6P1 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |
| 1xb2 | P43896-P49410 | 9913 | <i>Bos taurus</i> |
| 1xd3 | P15374-P15374-P62988-P62988 | 9606 | <i>Homo sapiens</i> |
| 1xd3 | P09936-P09936-P62988-P62988 | 9606 | <i>Homo sapiens</i> |
| 1xd3 | P09936-P09936-Q15843-Q15843 | 9606 | <i>Homo sapiens</i> |
| 1xew | P51834-P51834 | 224308 | <i>Bacillus subtilis</i> subsp. <i>subtilis</i> str. 168 |
| 1xew | O42649-O94383 | 4896 | <i>Schizosaccharomyces pombe</i> |
| 1xew | P41003-P41004 | 4896 | <i>Schizosaccharomyces pombe</i> |
| 1xew | P32908-P47037 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1xew | P32908-P38989 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1xew | P47037-P47037 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1xew | P47037-Q12267 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1xew | P38989-P47037 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1xew | Q09591-Q20060 | 6239 | <i>Caenorhabditis elegans</i> |
| 1xew | P48996-Q09591 | 6239 | <i>Caenorhabditis elegans</i> |
| 1xew | Q14683-Q9UQE7 | 9606 | <i>Homo sapiens</i> |
| 1xew | O95347-Q9NTJ3 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P30282-Q64261 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P30280-P30285 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P30282-P30285 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P25322-Q64261 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P25322-P30285 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P25322-P97377 | 10090 | <i>Mus musculus</i> |
| 1xo2 | P35426-Q04827 | 10116 | <i>Rattus norvegicus</i> |
| 1xo2 | P35426-P48961 | 10116 | <i>Rattus norvegicus</i> |
| 1xo2 | P35426-P39948 | 10116 | <i>Rattus norvegicus</i> |
| 1xo2 | P23573-P54733 | 7227 | <i>Drosophila melanogaster</i> |
| 1xo2 | P23572-Q9I7I0 | 7227 | <i>Drosophila melanogaster</i> |
| 1xo2 | P23572-P54733 | 7227 | <i>Drosophila melanogaster</i> |
| 1xo2 | P30281-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P11802-P30279 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P11802-P30281 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P24385-Q00534 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P24941-P30279 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P11802-P24385 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | O94921-P30281 | 9606 | <i>Homo sapiens</i> |
| 1xo2 | P24385-P24941 | 9606 | <i>Homo sapiens</i> |
| 1xq5 | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| 1xq5 | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| 1xq5 | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| 1xqs | P54652-P54652-Q9NZL4-Q9NZL4 | 9606 | <i>Homo sapiens</i> |
| 1xqs | P11142-P11142-Q9NZL4-Q9NZL4 | 9606 | <i>Homo sapiens</i> |
| 1xqs | P08107-P08107-Q9NZL4-Q9NZL4 | 9606 | <i>Homo sapiens</i> |
| 1xr8 | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 1xt9 | Q15843-Q96LD8 | 9606 | <i>Homo sapiens</i> |
| 1yl4 | P20433-P20433-P34087-P34087 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1y6n | P22301-Q13651 | 9606 | <i>Homo sapiens</i> |
| 1y8x | P61081-Q8TBC4 | 9606 | <i>Homo sapiens</i> |
| 1y96 | Q9CWX4-Q9CWX4-Q9CX53-Q9CX53 | 10090 | <i>Mus musculus</i> |
| 1y96 | Q8WXD5-Q8WXD5-Q9H840-Q9H840 | 9606 | <i>Homo sapiens</i> |
| 1ya5 | Q15273-Q8WZ42-Q8WZ42 | 9606 | <i>Homo sapiens</i> |
| 1yag | Q62468-Q9QZ83 | 10090 | <i>Mus musculus</i> |
| 1yag | P83967-Q24020 | 7227 | <i>Drosophila melanogaster</i> |
| 1yc0 | O43278-Q04756 | 9606 | <i>Homo sapiens</i> |
| 1yCS | P04637-Q13625 | 9606 | <i>Homo sapiens</i> |
| 1yd8 | P62988-P62988-Q9NZ52-Q9NZ52 | 9606 | <i>Homo sapiens</i> |
| 1yd8 | P62988-P62988-Q9UJY5-Q9UJY5 | 9606 | <i>Homo sapiens</i> |
| 1ykh | P47822-Q08278 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1ytf | P32773-P32773-P32774 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1yuk | P26010-P26010 | 9606 | <i>Homo sapiens</i> |
| 1yuk | P05556-P05556 | 9606 | <i>Homo sapiens</i> |
| 1zbd | P47708-P55258 | 10090 | <i>Mus musculus</i> |
| 1zbd | P47708-P63011 | 10090 | <i>Mus musculus</i> |
| 1zbd | P47708-Q9ERI2 | 10090 | <i>Mus musculus</i> |
| 1zbd | P47709-P63012 | 10116 | <i>Rattus norvegicus</i> |
| 1zbd | P41885-Q9NA29 | 6239 | <i>Caenorhabditis elegans</i> |
| 1ze3 | P08191-P30130-P31697 | 316407 | <i>Escherichia coli</i> str. K-12 substr. W3110 |
| 1ze3 | P08191-P30130-P31697 | 511145 | <i>Escherichia coli</i> str. K-12 substr. MG1655 |

Table S2. Gold standard positive set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|---|----------------|--|
| 1zhi | P06701-P21691 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 1zjd | P05067-Q92876 | 9606 | <i>Homo sapiens</i> |
| 2a5t | P35438-Q01097 | 10090 | <i>Mus musculus</i> |
| 2a5t | P35436-P35438 | 10090 | <i>Mus musculus</i> |
| 2a5t | P35438-P35438 | 10090 | <i>Mus musculus</i> |
| 2aa1 | P01942-P01942-P02089-P02089 | 10090 | <i>Mus musculus</i> |
| 2aa1 | P01942-P01942-P02088-P02088 | 10090 | <i>Mus musculus</i> |
| 2aa1 | P68871-P68871-P69905-P69905 | 9606 | <i>Homo sapiens</i> |
| 2aly | O26837-O26864 | 187420 | <i>Methanothermobacter thermautotrophicus str. Delta H</i> |
| 2aly | P07395-P08312 | 316407 | <i>Escherichia coli str. K-12 substr. W3110</i> |
| 2aly | P07395-P08312 | 511145 | <i>Escherichia coli str. K-12 substr. MG1655</i> |
| 2ast | P61024-P63208-Q13309 | 9606 | <i>Homo sapiens</i> |
| 2atc | P0A786-P0A7F3 | 316407 | <i>Escherichia coli str. K-12 substr. W3110</i> |
| 2atc | P0A786-P0A7F3 | 511145 | <i>Escherichia coli str. K-12 substr. MG1655</i> |
| 2b7d | P08709-P08709-P13726 | 9606 | <i>Homo sapiens</i> |
| 2bck | P07151-P07151-P13599-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 2be6 | O88751-O88751-O88751-P22002-P22002 -P22002 | 10116 | <i>Rattus norvegicus</i> |
| 2be6 | P62158-P62158-P62158-Q13936-Q13936 -Q13936 | 9606 | <i>Homo sapiens</i> |
| 2be6 | Q13936-Q13936-Q13936-Q9NZU7-Q9NZU7 -Q9NZU7 | 9606 | <i>Homo sapiens</i> |
| 2bki | P06787-Q04439 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 2bki | P62158-Q9UM54 | 9606 | <i>Homo sapiens</i> |
| 2bpt | P20676-Q06142 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 2btf | P35080-P63261 | 9606 | <i>Homo sapiens</i> |
| 2c0j | O43617-O75865 | 9606 | <i>Homo sapiens</i> |
| 2c7l | Q01951-Q54715 | 1148 | <i>Synechocystis sp. PCC 6803</i> |
| 2dhh | P01942-P02088 | 10090 | <i>Mus musculus</i> |
| 2dhh | P01942-P02089 | 10090 | <i>Mus musculus</i> |
| 2dhh | P68871-P69905 | 9606 | <i>Homo sapiens</i> |
| 2fif | P62988-P62988-P62988-Q9UJ41-Q9UJ41 -Q9UJ41 | 9606 | <i>Homo sapiens</i> |
| 2fwo | P07151-P13599 | 10116 | <i>Rattus norvegicus</i> |
| 2iad | P14434-P14483 | 10090 | <i>Mus musculus</i> |
| 3c98 | P32851-P61765 | 10116 | <i>Rattus norvegicus</i> |
| 3c98 | Q42374-Q9C5X3 | 3702 | <i>Arabidopsis thaliana</i> |
| 3c98 | Q07327-Q24547 | 7227 | <i>Drosophila melanogaster</i> |
| 3fhi | P06245-P07278 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 3fhi | P05986-P07278 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 3fhi | P06244-P07278 | 4932 | <i>Saccharomyces cerevisiae</i> |
| 3fhi | P21137-P30625 | 6239 | <i>Caenorhabditis elegans</i> |
| 3fhi | P12370-P81900 | 7227 | <i>Drosophila melanogaster</i> |
| 3fhi | P10644-P17612 | 9606 | <i>Homo sapiens</i> |
| 3gtu | P10299-P10299-P91505-P91505 | 6239 | <i>Caenorhabditis elegans</i> |
| 3qtu | P21266-P21266-P21266-P21266 | 9606 | <i>Homo sapiens</i> |

Table S3. Gold standard negative set

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|----------------------|
| 1a0r | P62880-Q61012-Q9QW08 | 10090 | Mus musculus |
| 1a0r | P61953-P62880-Q9QW08 | 10090 | Mus musculus |
| 1a0r | P62880-Q61017-Q9QW08 | 10090 | Mus musculus |
| lagr | Q4L0E8-Q4L0E8-Q9JID2-Q9JID2 | 10116 | Rattus norvegicus |
| lagr | O14924-O14924-P04899-P04899 | 9606 | Homo sapiens |
| laui | P48454-Q6PIL6 | 9606 | Homo sapiens |
| lava | Q8LFG1-Q8LFG1-Q8RXD5-Q8RXD5 | 3702 | Arabidopsis thaliana |
| lbqq | P48032-Q499S5 | 10116 | Rattus norvegicus |
| lbqq | A1EC81-P48032 | 10116 | Rattus norvegicus |
| lbqq | P07152-P48032 | 10116 | Rattus norvegicus |
| lbqq | C0M4B0-P48032 | 10116 | Rattus norvegicus |
| lbqq | B5DFD5-P48032 | 10116 | Rattus norvegicus |
| lbqq | P48032-P50280 | 10116 | Rattus norvegicus |
| lbqq | O88272-P48032 | 10116 | Rattus norvegicus |
| lbrc | O88301-Q61482 | 10090 | Mus musculus |
| lbrc | Q61482-Q91Y82 | 10090 | Mus musculus |
| lbrc | O88301-Q60709 | 10090 | Mus musculus |
| lbrc | Q60709-Q91Y82 | 10090 | Mus musculus |
| lbrc | P21845-Q61482 | 10090 | Mus musculus |
| lbrc | P21845-Q60709 | 10090 | Mus musculus |
| lbrc | Q60709-Q8K0D2 | 10090 | Mus musculus |
| lbrc | Q61482-Q8K0D2 | 10090 | Mus musculus |
| lbrc | Q61482-Q9QYN3 | 10090 | Mus musculus |
| lbrc | Q60709-Q9QYN3 | 10090 | Mus musculus |
| lbrc | Q60709-Q8VIF2 | 10090 | Mus musculus |
| lbrc | Q61482-Q8VIF2 | 10090 | Mus musculus |
| lbrc | Q60709-Q7M761 | 10090 | Mus musculus |
| lbrc | Q61482-Q7M761 | 10090 | Mus musculus |
| lbrc | Q60709-Q9R098 | 10090 | Mus musculus |
| lbrc | Q61482-Q9R098 | 10090 | Mus musculus |
| lbrc | Q61482-Q80WM7 | 10090 | Mus musculus |
| lbrc | Q60709-Q80WM7 | 10090 | Mus musculus |
| lbrc | Q61482-Q99MS4 | 10090 | Mus musculus |
| lbrc | Q60709-Q99MS4 | 10090 | Mus musculus |
| lbrc | Q60709-Q91VE3 | 10090 | Mus musculus |
| lbrc | Q61482-Q91VE3 | 10090 | Mus musculus |
| lbrc | Q5K2P8-Q61482 | 10090 | Mus musculus |
| lbrc | Q5K2P8-Q60709 | 10090 | Mus musculus |
| lbrc | P05208-Q61482 | 10090 | Mus musculus |
| lbrc | P05208-Q60709 | 10090 | Mus musculus |
| lbrc | Q14B25-Q61482 | 10090 | Mus musculus |
| lbrc | Q14B25-Q60709 | 10090 | Mus musculus |
| lbrc | Q3UKY7-Q61482 | 10090 | Mus musculus |
| lbrc | Q3UKY7-Q60709 | 10090 | Mus musculus |
| lbrc | Q571E5-Q61482 | 10090 | Mus musculus |
| lbrc | Q571E5-Q60709 | 10090 | Mus musculus |
| lbrc | Q61482-Q61759 | 10090 | Mus musculus |
| lbrc | Q60709-Q61759 | 10090 | Mus musculus |
| lbrc | Q14B24-Q60709 | 10090 | Mus musculus |
| lbrc | Q14B24-Q61482 | 10090 | Mus musculus |
| lbrc | Q60709-Q8BJR6 | 10090 | Mus musculus |
| lbrc | Q61482-Q8BJR6 | 10090 | Mus musculus |
| lbrc | Q60709-Q9D9G7 | 10090 | Mus musculus |
| lbrc | Q61482-Q9D9G7 | 10090 | Mus musculus |
| lbrc | P43430-Q60709 | 10090 | Mus musculus |
| lbrc | P43430-Q61482 | 10090 | Mus musculus |
| lbrc | Q61482-Q8K4I7 | 10090 | Mus musculus |
| lbrc | Q60709-Q8K4I7 | 10090 | Mus musculus |
| lbrc | Q61482-Q8BW11 | 10090 | Mus musculus |
| lbrc | Q60709-Q8BW11 | 10090 | Mus musculus |
| lbrc | Q60709-Q61646 | 10090 | Mus musculus |
| lbrc | P00762-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P00763-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P08426-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P27435-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P32822-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P32821-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P50343-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q6L711-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q5M879-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q5EBA7-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P00773-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q5K2P9-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P00774-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P18292-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P12788-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P31394-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P16296-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q5FVS2-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q6IE59-Q6P6Q5 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lbrc | Q6BEA2-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P09650-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P97594-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q6IE62-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P97592-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | P50339-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q6IE06-Q6P6Q5 | 10116 | Rattus norvegicus |
| lbrc | Q6P6Q5-Q6TUF8 | 10116 | Rattus norvegicus |
| lbrc | P07477-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q8NHM4 | 9606 | Homo sapiens |
| lbrc | Q06481-Q7Z5A4 | 9606 | Homo sapiens |
| lbrc | P20231-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q15661 | 9606 | Homo sapiens |
| lbrc | P35030-Q06481 | 9606 | Homo sapiens |
| lbrc | P40313-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q9UBX7 | 9606 | Homo sapiens |
| lbrc | Q06481-Q14520 | 9606 | Homo sapiens |
| lbrc | P08519-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q7RTZ1 | 9606 | Homo sapiens |
| lbrc | Q06481-Q9UKQ9 | 9606 | Homo sapiens |
| lbrc | Q06481-Q8NF86 | 9606 | Homo sapiens |
| lbrc | B4DNJ1-Q06481 | 9606 | Homo sapiens |
| lbrc | B4DN26-Q06481 | 9606 | Homo sapiens |
| lbrc | P00750-Q06481 | 9606 | Homo sapiens |
| lbrc | B4DV92-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q9UNI1 | 9606 | Homo sapiens |
| lbrc | Q06481-Q7RTY7 | 9606 | Homo sapiens |
| lbrc | A6NIE9-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q9H2R5 | 9606 | Homo sapiens |
| lbrc | P08217-Q06481 | 9606 | Homo sapiens |
| lbrc | O43240-Q06481 | 9606 | Homo sapiens |
| lbrc | Q04756-Q06481 | 9606 | Homo sapiens |
| lbrc | P17538-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q6GPI1 | 9606 | Homo sapiens |
| lbrc | A8MTI9-Q06481 | 9606 | Homo sapiens |
| lbrc | P49862-Q06481 | 9606 | Homo sapiens |
| lbrc | Q06481-Q7RTY5 | 9606 | Homo sapiens |
| lbrc | Q06481-Q9Y5K2 | 9606 | Homo sapiens |
| lcd9 | A2A8Y3-A2A8Y3-P09920-P09920 | 10090 | Mus musculus |
| lcd9 | P09920-P09920-P40223-P40223 | 10090 | Mus musculus |
| lcd9 | P09920-P09920-Q14BI3-Q14BI3 | 10090 | Mus musculus |
| lcd9 | P13854-P13854-Q5F3Y5-Q5F3Y5 | 9031 | Gallus gallus |
| lcd9 | P13854-P13854-Q9W6U9-Q9W6U9 | 9031 | Gallus gallus |
| lcul | P22717-P26769-P29348 | 10116 | Rattus norvegicus |
| lcul | P22717-P26770-P29348 | 10116 | Rattus norvegicus |
| lcul | P22717-P29348-Q66HK5 | 10116 | Rattus norvegicus |
| lcul | P22717-Q66HK5-Q9JID2 | 10116 | Rattus norvegicus |
| lcul | O75343-P04899-P51828 | 9606 | Homo sapiens |
| lcul | P04899-P33402-P51828 | 9606 | Homo sapiens |
| lcul | B7ZLX9-P04899-Q02108 | 9606 | Homo sapiens |
| lcul | P04899-P33402-Q4F7X0 | 9606 | Homo sapiens |
| lcul | O43306-P04899-P33402 | 9606 | Homo sapiens |
| lcul | B7Z8A6-P04899-P33402 | 9606 | Homo sapiens |
| lcul | B3KWA8-P04899-P33402 | 9606 | Homo sapiens |
| lcul | O60503-P04899-P33402 | 9606 | Homo sapiens |
| lcul | B7ZLX9-P50148-Q02108 | 9606 | Homo sapiens |
| lcul | B7ZLX9-P29992-Q02108 | 9606 | Homo sapiens |
| lcul | P33402-P50148-Q4F7X0 | 9606 | Homo sapiens |
| lcul | P29992-P33402-Q4F7X0 | 9606 | Homo sapiens |
| lcul | B7Z8A6-P29992-P33402 | 9606 | Homo sapiens |
| lcul | B3KWA8-P33402-P50148 | 9606 | Homo sapiens |
| lcul | B3KWA8-P29992-P33402 | 9606 | Homo sapiens |
| lcul | B7Z8A6-P33402-P50148 | 9606 | Homo sapiens |
| lcul | A5PKE5-P04695-P19687 | 9913 | Bos taurus |
| lcul | P04695-P19687-Q29450 | 9913 | Bos taurus |
| lcul | A5PKE5-P04695-P16068 | 9913 | Bos taurus |
| lcul | P04695-P16068-Q29450 | 9913 | Bos taurus |
| lcul | P04695-P19687-P19754 | 9913 | Bos taurus |
| ldfj | P34096-Q9C000 | 9606 | Homo sapiens |
| le96 | O70145-Q8BHH2 | 10090 | Mus musculus |
| le96 | O70145-Q9ROM6 | 10090 | Mus musculus |
| le96 | O70145-Q8K386 | 10090 | Mus musculus |
| le96 | O70145-P55258 | 10090 | Mus musculus |
| le96 | Q504M8-Q8CJ00 | 10090 | Mus musculus |
| levt | A4JYI8-A4JYI8-P48802-P48802 | 7955 | Danio rerio |
| levt | A4QN31-A4QN31-P48802-P48802 | 7955 | Danio rerio |
| levt | P48802-P48802-Q8AYP3-Q8AYP3 | 7955 | Danio rerio |
| levt | P48802-P48802-Q805B9-Q805B9 | 7955 | Danio rerio |
| levt | B4DVP5-B4DVP5-P08620-P08620 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| levt | P08620-P08620-Q59F30-Q59F30 | 9606 | Homo sapiens |
| levt | O43320-O43320-Q59F30-Q59F30 | 9606 | Homo sapiens |
| levt | B4DVP5-B4DVP5-O43320-O43320 | 9606 | Homo sapiens |
| levt | B4DVP5-B4DVP5-P31371-P31371 | 9606 | Homo sapiens |
| levt | P31371-P31371-Q59F30-Q59F30 | 9606 | Homo sapiens |
| levt | P12034-P12034-Q59F30-Q59F30 | 9606 | Homo sapiens |
| levt | B4DVP5-B4DVP5-P12034-P12034 | 9606 | Homo sapiens |
| levt | B4DVP5-B4DVP5-P11487-P11487 | 9606 | Homo sapiens |
| levt | P11487-P11487-Q59F30-Q59F30 | 9606 | Homo sapiens |
| levt | A0MTF4-A0MTF4-A4IFL5-A4IFL5 | 9913 | Bos taurus |
| levt | A0MTF4-A0MTF4-A7E310-A7E310 | 9913 | Bos taurus |
| lfle | B7Z459-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q8IU80 | 9606 | Homo sapiens |
| lfle | P19957-Q9BYE2 | 9606 | Homo sapiens |
| lfle | P19957-Q1RMF8 | 9606 | Homo sapiens |
| lfle | B7Z1L4-P19957 | 9606 | Homo sapiens |
| lfle | P05981-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q9NRS4 | 9606 | Homo sapiens |
| lfle | A8MYM4-P19957 | 9606 | Homo sapiens |
| lfle | B4DTM9-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q86WS5 | 9606 | Homo sapiens |
| lfle | B7WPR2-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q5USC7 | 9606 | Homo sapiens |
| lfle | P19957-P57727 | 9606 | Homo sapiens |
| lfle | P19957-Q9NRR2 | 9606 | Homo sapiens |
| lfle | P19957-Q9H3S3 | 9606 | Homo sapiens |
| lfle | P19957-Q86T26 | 9606 | Homo sapiens |
| lfle | P19957-Q7RTY9 | 9606 | Homo sapiens |
| lfle | P10323-P19957 | 9606 | Homo sapiens |
| lfle | P19957-P98073 | 9606 | Homo sapiens |
| lfle | P19957-Q9Y6M0 | 9606 | Homo sapiens |
| lfle | P19957-Q9Y5Y6 | 9606 | Homo sapiens |
| lfle | P19957-Q9Y5Q5 | 9606 | Homo sapiens |
| lfle | P19957-Q7RTY8 | 9606 | Homo sapiens |
| lfle | P08311-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q6UWB4 | 9606 | Homo sapiens |
| lfle | P19957-P20718 | 9606 | Homo sapiens |
| lfle | B4DRF2-P19957 | 9606 | Homo sapiens |
| lfle | P19957-Q7Z410 | 9606 | Homo sapiens |
| lfle | P10144-P19957 | 9606 | Homo sapiens |
| lfle | B7Z311-P19957 | 9606 | Homo sapiens |
| lfq1 | B2RZ50-P26817 | 10116 | Rattus norvegicus |
| lfq9 | P36363-P36363-Q3UQ28-Q3UQ28 | 10090 | Mus musculus |
| lfq9 | P48802-P48802-Q8AYP3-Q8AYP3 | 7955 | Danio rerio |
| lfq9 | A4QN31-A4QN31-P48802-P48802 | 7955 | Danio rerio |
| lfq9 | A4JYI8-A4JYI8-P48802-P48802 | 7955 | Danio rerio |
| lfq9 | P48802-P48802-Q805B9-Q805B9 | 7955 | Danio rerio |
| lfq9 | B4DVP5-B4DVP5-P10767-P10767 | 9606 | Homo sapiens |
| lfq9 | P10767-P10767-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | P08620-P08620-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-P08620-P08620 | 9606 | Homo sapiens |
| lfq9 | P12034-P12034-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-P12034-P12034 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-P31371-P31371 | 9606 | Homo sapiens |
| lfq9 | P31371-P31371-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | O43320-O43320-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-O43320-O43320 | 9606 | Homo sapiens |
| lfq9 | P11487-P11487-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-P11487-P11487 | 9606 | Homo sapiens |
| lfq9 | P55075-P55075-Q59F30-Q59F30 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-P55075-P55075 | 9606 | Homo sapiens |
| lfq9 | Q59F30-Q59F30-Q9HCT0-Q9HCT0 | 9606 | Homo sapiens |
| lfq9 | B4DVP5-B4DVP5-Q9HCT0-Q9HCT0 | 9606 | Homo sapiens |
| lfq9 | A0MTF4-A0MTF4-A4IFL5-A4IFL5 | 9913 | Bos taurus |
| lfq9 | A0MTF4-A0MTF4-A7E310-A7E310 | 9913 | Bos taurus |
| lg4y | B4YDY0-Q8VHC5 | 10090 | Mus musculus |
| lg4y | Q8VHC5-Q9EQR3 | 10090 | Mus musculus |
| lg4y | P58391-Q8VHC5 | 10090 | Mus musculus |
| lg4y | Q3UU99-Q8VHC5 | 10090 | Mus musculus |
| lg4y | Q6PJI0-Q9NP86 | 9606 | Homo sapiens |
| lg4y | Q6X2Y2-Q9NP86 | 9606 | Homo sapiens |
| lg4y | Q86VF9-Q9NP86 | 9606 | Homo sapiens |
| lg4y | Q6JXY2-Q9NP86 | 9606 | Homo sapiens |
| lg4y | Q8WVG7-Q9NP86 | 9606 | Homo sapiens |
| lg4y | O15554-Q9NP86 | 9606 | Homo sapiens |
| lgg2 | P04899-P59768-P62879 | 9606 | Homo sapiens |
| lgg2 | P04899-P62879-Q9UBI6 | 9606 | Homo sapiens |
| lgg2 | O60262-P04899-P62879 | 9606 | Homo sapiens |
| lgg2 | P29992-P62879-Q9UBI6 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|----------------------|----------------|-------------------|
| lgg2 | P04899-P62879-P63215 | 9606 | Homo sapiens |
| lgg2 | P50148-P62879-Q9UBI6 | 9606 | Homo sapiens |
| lgg2 | O60262-P29992-P62879 | 9606 | Homo sapiens |
| lgg2 | O60262-P50148-P62879 | 9606 | Homo sapiens |
| lgg2 | P29992-P62879-P63215 | 9606 | Homo sapiens |
| lgg2 | P04899-P50150-P62879 | 9606 | Homo sapiens |
| lgg2 | P50148-P62879-P63215 | 9606 | Homo sapiens |
| lgg2 | P29992-P50150-P62879 | 9606 | Homo sapiens |
| lgg2 | P50148-P50150-P62879 | 9606 | Homo sapiens |
| lgg2 | P04899-P62879-Q9UK08 | 9606 | Homo sapiens |
| lgg2 | P29992-P62879-Q9UK08 | 9606 | Homo sapiens |
| lgg2 | P50148-P62879-Q9UK08 | 9606 | Homo sapiens |
| lgot | P04899-P62879-P63211 | 9606 | Homo sapiens |
| lgot | P04899-P61952-P62879 | 9606 | Homo sapiens |
| lgot | P50148-P62879-P63211 | 9606 | Homo sapiens |
| lgot | P50148-P61952-P62879 | 9606 | Homo sapiens |
| lgot | P29992-P62879-P63211 | 9606 | Homo sapiens |
| lgot | P29992-P61952-P62879 | 9606 | Homo sapiens |
| lgot | O14610-P04899-P62879 | 9606 | Homo sapiens |
| lgot | O14610-P50148-P62879 | 9606 | Homo sapiens |
| lgot | O14610-P29992-P62879 | 9606 | Homo sapiens |
| lj9c | P20352-P70375-Q9D9M0 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q61646 | 10090 | Mus musculus |
| lj9c | P20352-P70375-P97435 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q5S248 | 10090 | Mus musculus |
| lj9c | O70169-P20352-P70375 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q8BIK6 | 10090 | Mus musculus |
| lj9c | P20352-P56677-P70375 | 10090 | Mus musculus |
| lj9c | B2RY54-P20352-P70375 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q14C59 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q8BU25 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q80UR4 | 10090 | Mus musculus |
| lj9c | P20352-P70375-Q9QYZ9 | 10090 | Mus musculus |
| lj9c | P42533-P69526-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P69526-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P42533-P86091-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P86091-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | Q66HI4-Q8K3U6-Q9JJI7 | 10116 | Rattus norvegicus |
| lj9c | P42533-Q8K3U6-Q9JJI7 | 10116 | Rattus norvegicus |
| lj9c | P83748-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P42533-P83748-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P42533-Q6IE14-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | Q66HI4-Q6IE14-Q8K3U6 | 10116 | Rattus norvegicus |
| lj9c | P00739-P08709-Q86WH4 | 9606 | Homo sapiens |
| lj9c | P08709-Q2TV78-Q86WH4 | 9606 | Homo sapiens |
| lj9c | P08709-Q5K4E3-Q86WH4 | 9606 | Homo sapiens |
| lj9c | P08709-Q86WH4-Q9GZN4 | 9606 | Homo sapiens |
| lj9c | P08709-Q7RTY7-Q86WH4 | 9606 | Homo sapiens |
| lj9c | P22457-P30931-P98072 | 9913 | Bos taurus |
| lj9c | P22457-P30931-Q5E9P5 | 9913 | Bos taurus |
| lj9c | P22457-P30931-QOIIH7 | 9913 | Bos taurus |
| ljrh | P01610-P04438-P15260 | 9606 | Homo sapiens |
| ljrh | P04207-P04438-P15260 | 9606 | Homo sapiens |
| ljrh | P04438-P06314-P15260 | 9606 | Homo sapiens |
| ljrh | P01594-P04438-P15260 | 9606 | Homo sapiens |
| ljrh | P01610-P01761-P15260 | 9606 | Homo sapiens |
| ljrh | P01761-P06314-P15260 | 9606 | Homo sapiens |
| ljrh | P01761-P04207-P15260 | 9606 | Homo sapiens |
| ljrh | P01594-P01761-P15260 | 9606 | Homo sapiens |
| ljrh | P01610-P01816-P15260 | 9606 | Homo sapiens |
| ljrh | P01610-P01771-P15260 | 9606 | Homo sapiens |
| ljrh | P01816-P04207-P15260 | 9606 | Homo sapiens |
| ljrh | P01816-P06314-P15260 | 9606 | Homo sapiens |
| ljrh | P01594-P01816-P15260 | 9606 | Homo sapiens |
| ljrh | P01771-P04207-P15260 | 9606 | Homo sapiens |
| ljrh | P01594-P01771-P15260 | 9606 | Homo sapiens |
| ljrh | P01771-P06314-P15260 | 9606 | Homo sapiens |
| ljsu | O08769-Q2PYT3-Q6AY13 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q69DC0-Q6GX89 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q69DC0-Q6GX88 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q69DC1-Q6AY13 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q69DC0-Q6AY13 | 10116 | Rattus norvegicus |
| ljsu | O08769-Q2PYT3-Q5M857 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q5M857-Q69DC1 | 10116 | Rattus norvegicus |
| ljsu | Q2PYT3-Q5M857-Q69DC0 | 10116 | Rattus norvegicus |
| ljsu | P30277-Q2PYT3-Q69DC0 | 10116 | Rattus norvegicus |
| ljsu | B1WC54-O08769-Q2PYT3 | 10116 | Rattus norvegicus |
| ljsu | P39949-Q2PYT3-Q69DC0 | 10116 | Rattus norvegicus |
| ljsu | B1WC54-Q2PYT3-Q69DC0 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|----------------------|----------------|-------------------|
| 1jsu | B1WC54-Q2PYT3-Q69DC1 | 10116 | Rattus norvegicus |
| 1jsu | P46527-P78396-Q8TD08 | 9606 | Homo sapiens |
| 1jsu | B7Z7E3-P46527-Q8TD08 | 9606 | Homo sapiens |
| 1jsu | P20248-P46527-Q8TD08 | 9606 | Homo sapiens |
| 1jsu | P46527-Q5TZP9-Q8TD08 | 9606 | Homo sapiens |
| 1jsu | Q95067-P46527-Q8TD08 | 9606 | Homo sapiens |
| 1jsu | P46527-Q8TD08-Q8WWL7 | 9606 | Homo sapiens |
| 1jsu | A4IFL5-A6QLS3-P30274 | 9913 | Bos taurus |
| 1jsu | A4IFL5-P30274-Q08DQ5 | 9913 | Bos taurus |
| 1k9o | P23578-Q03734 | 10090 | Mus musculus |
| 1k9o | Q07235-Q9D9M0 | 10090 | Mus musculus |
| 1k9o | Q03734-Q3TZ06 | 10090 | Mus musculus |
| 1k9o | Q03734-Q812A6 | 10090 | Mus musculus |
| 1k9o | Q03734-Q8VCA5 | 10090 | Mus musculus |
| 1k9o | Q03734-Q14BX2 | 10090 | Mus musculus |
| 1k9o | Q07235-Q9QYZ9 | 10090 | Mus musculus |
| 1k9o | Q07235-Q14BX2 | 10090 | Mus musculus |
| 1k9o | Q07235-Q812A6 | 10090 | Mus musculus |
| 1k9o | Q07235-Q3TZ06 | 10090 | Mus musculus |
| 1k9o | Q03734-Q9QYZ9 | 10090 | Mus musculus |
| 1k9o | Q03734-Q9ER04 | 10090 | Mus musculus |
| 1k9o | Q07235-Q9ER04 | 10090 | Mus musculus |
| 1k9o | P97435-Q03734 | 10090 | Mus musculus |
| 1k9o | Q07235-Q8VCA5 | 10090 | Mus musculus |
| 1k9o | P23578-Q00897 | 10090 | Mus musculus |
| 1k9o | Q07235-Q5U405 | 10090 | Mus musculus |
| 1k9o | Q00897-Q9QYZ9 | 10090 | Mus musculus |
| 1k9o | Q03734-Q9D9M0 | 10090 | Mus musculus |
| 1k9o | Q07235-Q3UKE3 | 10090 | Mus musculus |
| 1k9o | Q07235-Q9DBI0 | 10090 | Mus musculus |
| 1k9o | B2RSC4-Q03734 | 10090 | Mus musculus |
| 1k9o | Q03734-Q3U0U6 | 10090 | Mus musculus |
| 1k9o | Q03734-Q9DBI0 | 10090 | Mus musculus |
| 1k9o | Q03734-Q3UKE3 | 10090 | Mus musculus |
| 1k9o | P97435-Q07235 | 10090 | Mus musculus |
| 1k9o | Q03734-Q5U405 | 10090 | Mus musculus |
| 1k9o | Q00897-Q3UKE3 | 10090 | Mus musculus |
| 1k9o | Q03734-Q3V0Q7 | 10090 | Mus musculus |
| 1k9o | Q00897-Q8VCA5 | 10090 | Mus musculus |
| 1k9o | Q00897-Q812A6 | 10090 | Mus musculus |
| 1k9o | Q00897-Q3TZ06 | 10090 | Mus musculus |
| 1k9o | Q00897-Q14BX2 | 10090 | Mus musculus |
| 1k9o | Q00897-Q9D9M0 | 10090 | Mus musculus |
| 1k9o | P97435-Q00897 | 10090 | Mus musculus |
| 1k9o | Q00897-Q5U405 | 10090 | Mus musculus |
| 1k9o | Q03734-Q9QUL7 | 10090 | Mus musculus |
| 1k9o | Q07235-Q920S2 | 10090 | Mus musculus |
| 1k9o | Q00897-Q9ER04 | 10090 | Mus musculus |
| 1k9o | B2RSC4-Q00897 | 10090 | Mus musculus |
| 1k9o | Q00897-Q3U0U6 | 10090 | Mus musculus |
| 1k9o | Q07235-Q9QUL7 | 10090 | Mus musculus |
| 1k9o | Q00897-Q9DBI0 | 10090 | Mus musculus |
| 1k9o | Q14BX2-Q91WP6 | 10090 | Mus musculus |
| 1k9o | Q68FT8-Q8CJ16 | 10116 | Rattus norvegicus |
| 1k9o | Q68FT8-Q8CJ17 | 10116 | Rattus norvegicus |
| 1k9o | P83748-Q68FT8 | 10116 | Rattus norvegicus |
| 1k9o | B2RYJ5-Q68FT8 | 10116 | Rattus norvegicus |
| 1k9o | P17475-Q05511 | 10116 | Rattus norvegicus |
| 1k9o | Q68FT8-Q6P7D7 | 10116 | Rattus norvegicus |
| 1k9o | P17475-P83748 | 10116 | Rattus norvegicus |
| 1k9o | P17475-Q8CJ17 | 10116 | Rattus norvegicus |
| 1k9o | P17475-Q8CJ16 | 10116 | Rattus norvegicus |
| 1k9o | P83748-Q5M7T5 | 10116 | Rattus norvegicus |
| 1k9o | P17475-Q6GQQ3 | 10116 | Rattus norvegicus |
| 1k9o | Q5M7T5-Q6P7D7 | 10116 | Rattus norvegicus |
| 1k9o | P17475-Q6P7D7 | 10116 | Rattus norvegicus |
| 1k9o | Q5M7T5-Q8CJ17 | 10116 | Rattus norvegicus |
| 1k9o | Q5M7T5-Q8CJ16 | 10116 | Rattus norvegicus |
| 1k9o | B2RYJ5-Q5M7T5 | 10116 | Rattus norvegicus |
| 1k9o | P86091-Q68FT8 | 10116 | Rattus norvegicus |
| 1k9o | B2RYJ5-P17475 | 10116 | Rattus norvegicus |
| 1k9o | Q05511-Q5M7T5 | 10116 | Rattus norvegicus |
| 1k9o | P83748-Q9JLD2 | 10116 | Rattus norvegicus |
| 1k9o | Q73790-Q90627 | 9031 | Gallus gallus |
| 1k9o | Q73790-Q90628 | 9031 | Gallus gallus |
| 1k9o | Q73790-Q90629 | 9031 | Gallus gallus |
| 1k9o | Q73790-P25155 | 9031 | Gallus gallus |
| 1k9o | Q73790-P15120 | 9031 | Gallus gallus |
| 1k9o | Q73790-Q91001 | 9031 | Gallus gallus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-----------------------------|
| 1k9o | O73790-Q804X5 | 9031 | Gallus gallus |
| 1k9o | O73790-Q804X7 | 9031 | Gallus gallus |
| 1k9o | P07477-P08697 | 9606 | Homo sapiens |
| 1k9o | P08697-Q8NHM4 | 9606 | Homo sapiens |
| 1k9o | B4DN26-P08697 | 9606 | Homo sapiens |
| 1k9o | B4DNJ1-P08697 | 9606 | Homo sapiens |
| 1k9o | B4DV92-P08697 | 9606 | Homo sapiens |
| 1k9o | P00747-Q9UIV8 | 9606 | Homo sapiens |
| 1k9o | P28800-P79343 | 9913 | Bos taurus |
| 1k9o | P28800-Q0IIH7 | 9913 | Bos taurus |
| 1k9o | A7E330-P28800 | 9913 | Bos taurus |
| 1k9o | A6QPX2-P28800 | 9913 | Bos taurus |
| 1k9o | A1L5C6-P28800 | 9913 | Bos taurus |
| 1k9o | A2VDV7-P28800 | 9913 | Bos taurus |
| 1k9o | A7E330-P41361 | 9913 | Bos taurus |
| 1k9o | A2VDV7-P41361 | 9913 | Bos taurus |
| 1k9o | P41361-Q0IIH7 | 9913 | Bos taurus |
| 1k9o | P28800-P98072 | 9913 | Bos taurus |
| 1k9o | A6QPX2-P41361 | 9913 | Bos taurus |
| 1k9o | P41361-P98072 | 9913 | Bos taurus |
| 1k9o | P28800-Q32PI4 | 9913 | Bos taurus |
| 1k9o | A7E330-P50448 | 9913 | Bos taurus |
| 1ktz | A8E7N9-Q58EQ1 | 7955 | Danio rerio |
| 1ktz | A1L1T8-Q58EQ1 | 7955 | Danio rerio |
| 1ktz | A8E7N9-B0S5M2 | 7955 | Danio rerio |
| 1ktz | Q58EQ1-Q8QGE3 | 7955 | Danio rerio |
| 1ktz | A1L1T8-B0S5M2 | 7955 | Danio rerio |
| 1ktz | B0S5M2-Q8QGE3 | 7955 | Danio rerio |
| 1ktz | Q90999-Q9I8T6 | 9031 | Gallus gallus |
| 1ktz | O42220-Q90999 | 9031 | Gallus gallus |
| 1ktz | B1AKZ9-P37173 | 9606 | Homo sapiens |
| 1ktz | Q4SUT7-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| 1ktz | Q4S1Z3-Q4SUT7 | 99883 | Tetraodon nigroviridis |
| 1ktz | Q4S0V9-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| 1ktz | Q4S0V9-Q4S1Z3 | 99883 | Tetraodon nigroviridis |
| lnf3 | Q5BJV7-Q5BJV7-Q6B4M5-Q6B4M5 | 10116 | Rattus norvegicus |
| lnpe | P02468-Q91ZX7 | 10090 | Mus musculus |
| lnpe | Q91ZX7-Q9R0B6 | 10090 | Mus musculus |
| lnpe | Q4VAI3-Q91ZX7 | 10090 | Mus musculus |
| lnpe | B1AXJ3-Q9R0B6 | 10090 | Mus musculus |
| lnpe | B1AXJ3-Q4VAI3 | 10090 | Mus musculus |
| lnpe | B1AXJ7-Q9R0B6 | 10090 | Mus musculus |
| lnpe | B1AXJ7-Q4VAI3 | 10090 | Mus musculus |
| lnpe | B1AXJ6-Q9R0B6 | 10090 | Mus musculus |
| lnpe | B1AXJ6-Q4VAI3 | 10090 | Mus musculus |
| lnpe | B1AXJ5-Q9R0B6 | 10090 | Mus musculus |
| lnpe | B1AXJ5-Q4VAI3 | 10090 | Mus musculus |
| lnpe | B1AXJ4-Q9R0B6 | 10090 | Mus musculus |
| lnpe | B1AXJ4-Q4VAI3 | 10090 | Mus musculus |
| lnpe | P02468-Q3TVR4 | 10090 | Mus musculus |
| lnpe | P02468-Q3TDD1 | 10090 | Mus musculus |
| lnpe | Q3TVR4-Q4VAI3 | 10090 | Mus musculus |
| lnpe | Q3TVR4-Q9R0B6 | 10090 | Mus musculus |
| lnpe | Q3TDD1-Q9R0B6 | 10090 | Mus musculus |
| lnpe | Q3TDD1-Q4VAI3 | 10090 | Mus musculus |
| lnpe | P97927-Q3TDD1 | 10090 | Mus musculus |
| lnpe | P97927-Q3TVR4 | 10090 | Mus musculus |
| lnpe | Q7PV65-Q7QJR9 | 180454 | Anopheles gambiae str. PEST |
| lnpe | B0S8G1-Q2Q1W5 | 7955 | Danio rerio |
| lnpe | Q5ZKF9-Q90ZN3 | 9031 | Gallus gallus |
| lnpe | O57484-Q98931 | 9031 | Gallus gallus |
| lnpe | O57484-P98157 | 9031 | Gallus gallus |
| lnpe | B1APY0-P01133 | 9606 | Homo sapiens |
| lnun | P13595-Q9ESL9 | 10090 | Mus musculus |
| lnun | O54769-O55005 | 10116 | Rattus norvegicus |
| lnun | P48802-Q805B9 | 7955 | Danio rerio |
| lnun | A4QN31-P48802 | 7955 | Danio rerio |
| lnun | P48802-Q8AYP3 | 7955 | Danio rerio |
| lnun | A4JYI8-P48802 | 7955 | Danio rerio |
| lnun | Q59F30-Q9HCT0 | 9606 | Homo sapiens |
| lnun | B4DVP5-Q9HCT0 | 9606 | Homo sapiens |
| lnun | B4DVP5-P10767 | 9606 | Homo sapiens |
| lnun | P10767-Q59F30 | 9606 | Homo sapiens |
| lnun | P31371-Q59F30 | 9606 | Homo sapiens |
| lnun | B4DVP5-P31371 | 9606 | Homo sapiens |
| lnun | O43320-Q59F30 | 9606 | Homo sapiens |
| lnun | B4DVP5-O43320 | 9606 | Homo sapiens |
| lnun | B4DVP5-P11487 | 9606 | Homo sapiens |
| lnun | P11487-Q59F30 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|----------------------|
| lnun | B4DVP5-P08620 | 9606 | Homo sapiens |
| lnun | P08620-Q59F30 | 9606 | Homo sapiens |
| lnun | P12034-Q59F30 | 9606 | Homo sapiens |
| lnun | B4DVP5-P12034 | 9606 | Homo sapiens |
| lnun | A0MTF4-A7E310 | 9913 | Bos taurus |
| lo5f | P07338-Q6GQQ3 | 10116 | Rattus norvegicus |
| loc0 | P04004-Q9UIV8 | 9606 | Homo sapiens |
| loc0 | P04004-Q96P63 | 9606 | Homo sapiens |
| loiu | Q9FMH5-Q9FMH5-Q9ZVM9-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| loph | Q07235-Q9D9M0 | 10090 | Mus musculus |
| loph | Q07235-Q3TZ06 | 10090 | Mus musculus |
| loph | Q07235-Q812A6 | 10090 | Mus musculus |
| loph | Q07235-Q9QYZ9 | 10090 | Mus musculus |
| loph | Q07235-Q8VCA5 | 10090 | Mus musculus |
| loph | P97435-Q07235 | 10090 | Mus musculus |
| loph | Q07235-Q9ER04 | 10090 | Mus musculus |
| loph | Q07235-Q3UKE3 | 10090 | Mus musculus |
| loph | P97435-Q00897 | 10090 | Mus musculus |
| loph | Q07235-Q9DBI0 | 10090 | Mus musculus |
| loph | Q07235-Q5U405 | 10090 | Mus musculus |
| loph | Q07235-Q3V0Q7 | 10090 | Mus musculus |
| loph | Q00897-Q9DBI0 | 10090 | Mus musculus |
| loph | Q00896-Q9DBI0 | 10090 | Mus musculus |
| loph | Q00896-Q8VCA5 | 10090 | Mus musculus |
| loph | P97435-Q00896 | 10090 | Mus musculus |
| loph | Q07235-Q14BX2 | 10090 | Mus musculus |
| loph | Q00896-Q9D9M0 | 10090 | Mus musculus |
| loph | Q00897-Q9QYZ9 | 10090 | Mus musculus |
| loph | Q00896-Q9QYZ9 | 10090 | Mus musculus |
| loph | Q00897-Q9D9M0 | 10090 | Mus musculus |
| loph | P23578-Q00897 | 10090 | Mus musculus |
| loph | Q00897-Q8VCA5 | 10090 | Mus musculus |
| loph | Q00897-Q3TZ06 | 10090 | Mus musculus |
| loph | Q00897-Q812A6 | 10090 | Mus musculus |
| loph | P23578-Q00896 | 10090 | Mus musculus |
| loph | Q00897-Q5U405 | 10090 | Mus musculus |
| loph | P00763-P29457 | 10116 | Rattus norvegicus |
| loph | P08426-P29457 | 10116 | Rattus norvegicus |
| loph | P00762-P29457 | 10116 | Rattus norvegicus |
| loph | P29457-Q5K2P9 | 10116 | Rattus norvegicus |
| loph | P29457-Q6L711 | 10116 | Rattus norvegicus |
| loph | P07092-P83748 | 10116 | Rattus norvegicus |
| loph | P07092-Q8CJ16 | 10116 | Rattus norvegicus |
| loph | P07092-Q8CJ17 | 10116 | Rattus norvegicus |
| loph | P07092-Q6P7D7 | 10116 | Rattus norvegicus |
| loph | B2RYJ5-P07092 | 10116 | Rattus norvegicus |
| loph | P29457-P50343 | 10116 | Rattus norvegicus |
| loph | P27435-P29457 | 10116 | Rattus norvegicus |
| loph | P19637-Q5RJR9 | 10116 | Rattus norvegicus |
| loph | P29457-Q5EBA7 | 10116 | Rattus norvegicus |
| loph | P29457-P32821 | 10116 | Rattus norvegicus |
| loph | P29457-P32822 | 10116 | Rattus norvegicus |
| loph | P00774-P29457 | 10116 | Rattus norvegicus |
| loph | P00773-P29457 | 10116 | Rattus norvegicus |
| loph | P07092-Q80YN4 | 10116 | Rattus norvegicus |
| loph | P17475-Q05511 | 10116 | Rattus norvegicus |
| loph | P07092-P86091 | 10116 | Rattus norvegicus |
| loph | P09650-P29457 | 10116 | Rattus norvegicus |
| loph | P12788-P29457 | 10116 | Rattus norvegicus |
| loph | P17475-Q8CJ17 | 10116 | Rattus norvegicus |
| loph | P17475-Q8CJ16 | 10116 | Rattus norvegicus |
| loph | P29457-Q6BEA2 | 10116 | Rattus norvegicus |
| loph | P17475-P83748 | 10116 | Rattus norvegicus |
| loph | P29457-P50339 | 10116 | Rattus norvegicus |
| loph | B2RYJ5-P17475 | 10116 | Rattus norvegicus |
| loph | P07092-P69526 | 10116 | Rattus norvegicus |
| loph | P17475-Q6P7D7 | 10116 | Rattus norvegicus |
| loph | P17475-Q80YN4 | 10116 | Rattus norvegicus |
| loph | P29457-P97594 | 10116 | Rattus norvegicus |
| loph | P50454-Q8NHM4 | 9606 | Homo sapiens |
| loph | P07477-P50454 | 9606 | Homo sapiens |
| loph | P35030-P50454 | 9606 | Homo sapiens |
| loph | B4DN87-P00747 | 9606 | Homo sapiens |
| loph | P20231-P50454 | 9606 | Homo sapiens |
| loph | P50454-Q15661 | 9606 | Homo sapiens |
| loph | P50454-Q14520 | 9606 | Homo sapiens |
| loph | P08519-P50454 | 9606 | Homo sapiens |
| loph | P50454-Q9P0G3 | 9606 | Homo sapiens |
| loph | P50454-Q9UBX7 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| loph | P50454-Q9Y337 | 9606 | Homo sapiens |
| loph | P40313-P50454 | 9606 | Homo sapiens |
| loph | P50454-Q9Y5K2 | 9606 | Homo sapiens |
| loph | P50454-Q7Z5A4 | 9606 | Homo sapiens |
| lpvh | P17777-P17777-P40190-P40190 | 10116 | Rattus norvegicus |
| lpyt | P28293-Q504N0-Q8R4H4-Q9CR35 | 10090 | Mus musculus |
| lpyt | P05208-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q3UN88-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P21812-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | A6H6T1-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q3UN88-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P21812-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q9CR35 | 10090 | Mus musculus |
| lpyt | P07146-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q8BIK6-Q8R4H4 | 10090 | Mus musculus |
| lpyt | A6H6T1-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q9CR35 | 10090 | Mus musculus |
| lpyt | P28293-P56677-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P07146-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q8R4H4-Q9R098 | 10090 | Mus musculus |
| lpyt | P19221-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P05208-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | A6H6T1-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q8R4H4-Q91Y82 | 10090 | Mus musculus |
| lpyt | O88301-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P05208-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q9R098 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q9R098 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q8R4H4-Q9JIQ8 | 10090 | Mus musculus |
| lpyt | P28293-Q3UKE3-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q61955-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P26928-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-P56677-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P21812-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q3UN88-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | B2RSC4-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q3U0U6-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q9CR35-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-P43430-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-P43430-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P07146-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q91Y82 | 10090 | Mus musculus |
| lpyt | O88301-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P26928-P28293-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q6P8K8-Q9CR35 | 10090 | Mus musculus |
| lpyt | P28293-Q14B24-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q3U0U6-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | B2RSC4-P28293-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-P56677-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q8BIK6 | 10090 | Mus musculus |
| lpyt | O88301-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q91Y82 | 10090 | Mus musculus |
| lpyt | A6H6T1-P28293-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-Q3U0U6-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | B2RSC4-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | O35727-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q14B24-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q61759-Q8R4H4 | 10090 | Mus musculus |
| lpyt | B2RSC4-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q3U0U6-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q9JHH6-Q9R098 | 10090 | Mus musculus |
| lpyt | P19221-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q61955 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q7M761 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q61759 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q8BIK6 | 10090 | Mus musculus |
| lpyt | P19221-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q8R4H4-Q9QYN3 | 10090 | Mus musculus |
| lpyt | P28293-Q14B24-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | A6H6T1-P28293-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | B2RSC4-P28293-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | P28293-Q3U0U6-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q61759 | 10090 | Mus musculus |
| lpyt | P06869-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P05208-P28293-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-Q3UKE3-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q5U901-Q9JIQ8 | 10090 | Mus musculus |
| lpyt | P28293-Q3UN88-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | P21812-P28293-Q504N0-Q6P8K8 | 10090 | Mus musculus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P28293-P43430-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | O35727-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-P56677-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q9QYN3 | 10090 | Mus musculus |
| lpyt | P06869-P28293-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P26928-P28293-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P26928-P28293-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P05208-P28293-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q504N0-Q9JIQ8 | 10090 | Mus musculus |
| lpyt | P28293-Q3UKE3-Q504N0-Q504N0 | 10090 | Mus musculus |
| lpyt | P28293-Q14B25-Q504N0-Q8R4H4 | 10090 | Mus musculus |
| lpyt | P28293-Q14B25-Q504N0-Q5U901 | 10090 | Mus musculus |
| lpyt | P28293-Q3UN88-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P21812-P28293-Q504N0-Q9JHH6 | 10090 | Mus musculus |
| lpyt | P28293-Q504N0-Q6P8K8-Q9R098 | 10090 | Mus musculus |
| lpyt | P26928-P28293-Q504N0-Q6P8K8 | 10090 | Mus musculus |
| lpyt | P00731-P00731-P00774-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00773-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q6IE62 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6IE62 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P36376-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q6BEA2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P50339 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P32822-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P32821-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | B2RYJ5-P00731-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q6L711 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P18292 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P29293 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q9WUW3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P50339 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6L711 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6BEA2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q9EQV9-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q99JC8 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6P7D7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P83748 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P36376-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P97592-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q8CJ17 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q8CJ16 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P09650 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00773-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q63207 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P18292-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00762-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P18292-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P09650-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q9EQV9-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q8K3U6 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-Q9EQV9-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00762-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6AXZ6 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P00731-P19637-P97594-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P12788 | 10116 | Rattus norvegicus |
| lpyt | P00774-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P08426 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P18292-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P12788-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00774-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | B2RYJ5-P07338-P19222-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-P29293 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9WUW3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q05511-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6IE62 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q6P7D7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P86091-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P08426-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q6IE59-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | B2RYJ5-P00731-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P31394 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q6AXZ6-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q9ES87 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q6P7D7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-P83748 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q6IE62 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00773-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q6GQQ3-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6IE62 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q8VHJ4-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6BEA2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P07338-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P29293 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P86091 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q8CJ17 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q8CJ16 | 10116 | Rattus norvegicus |
| lpyt | B2RYJ5-P07338-P19222-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P50339 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P31394 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P50343 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-P29293 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6L711 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P83748 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P18292-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6AXZ6 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q99JC8 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P36376-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6P7D7 | 10116 | Rattus norvegicus |
| lpyt | B2RYJ5-P07338-P19222-P21961 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P00731-P07338-P19222-P50343 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-Q05511-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P36376-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19222-P19637-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q6BEA2 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P29293 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-Q6P7D7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P86091-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9WUW3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P50339 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P50339 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6L711 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6BEA2 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P32821-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P32822-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q8CJ17 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q8CJ16 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q6L711 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P12788-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P18292-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q6P7D7 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19223-P19637-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-P83748 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P86091 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-Q6GQQ3-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P32822 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q9EQV9-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P32821 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q8CJ17 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q8CJ16 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P29598 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-Q9EQV9-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q99JC8 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6P7D7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-P36376 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P83748 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P09650-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q6AXZ6 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q63207 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q8CJ16 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q8CJ17 | 10116 | Rattus norvegicus |
| lpyt | P00731-P18292-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q8K3U6 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P36376 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P29598-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q63207 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5K2P9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P18292-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P97592-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19222-P19637-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P09650-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P09650-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P12788-P19222-P19637 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P07338-P19222-P21961-Q8K3U6 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00773-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q5EBA7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P18292-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P12788-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P18292 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00763-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q9EQV9-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6AXZ6 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19223-P19637-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00762-P07338 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P00731-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q6AXZ6 | 10116 | Rattus norvegicus |
| lpyt | P00762-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P08426-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P97594-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9ES87 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P12788-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00774-P19222-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P12788-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P29598 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19222-P19637-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P07338-P12788-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5K2P9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P08426-P21961 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P00774-P07338 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19223-P19637-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P08426-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P31394 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q05511-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-Q05511-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q6P7D7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P86091-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9ES87 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q01177 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q5M879-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-Q6P7D7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P86091-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P31394 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q6IE59-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P50343 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q6AXZ6-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P36376 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19223-P19637-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q6GQQ3-Q9EQV9 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P00731-P07338-P19222-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-Q6GQQ3-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q8VHJ4-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19222-P19637-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P50343 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P31394 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P50343 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00763-P07338-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-Q03238-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00762-P19222-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P29598 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-P36376 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P19223-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P12788-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P12788 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P86091 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q01177 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q5K2P9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P29598 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P69526 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6AXZ6 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5FVS2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-P29598 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P18292-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00763-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P29598-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00774-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q5K2P9 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00773-P19222-P19637-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q01177 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q5EBA7-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00763-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P69526 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-P97592 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-P29598 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P29598 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q5K2P9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P19223-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P12788-Q9EQV9 | 10116 | Rattus norvegicus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| lpyt | P00731-P08426-P19637-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5FVS2 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19223-Q01177 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5M879 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P19223-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9Z1D3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P19222-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q01177 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | O88780-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00762-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q5M879-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q5EBA7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P00763-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | O88780-P00731-P07338-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q05511 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-Q03238-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00774-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00773-P07338-P19222-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-P32821 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q5FVS2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P69526 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P21961 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P32821 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P32822 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-P29598 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P29598 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P19637-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-P97592 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19222-P19637-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19223-P19637-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q5FVS2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00773-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P08426-Q9EQV9 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P21961-Q5FVS2 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00762-P07338-P19223 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q8VHJ4 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P08426-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q6GQQ3 | 10116 | Rattus norvegicus |
| lpyt | P00731-P08426-P19222-P19637 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19222-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-Q03238 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P19223-Q6IE59 | 10116 | Rattus norvegicus |
| lpyt | P00731-P07338-P08426-P19222 | 10116 | Rattus norvegicus |
| lpyt | P00731-P00731-P07338-P08426 | 10116 | Rattus norvegicus |
| lpyt | P00731-P19637-P21961-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P19222-P19637-P21961-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P07338-P19222-P21961-Q9JJI7 | 10116 | Rattus norvegicus |
| lpyt | P00747-P15085-P15085-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-P15085 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-P15085 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8WXQ8-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7RTY8-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P48052-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-Q9UI42 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-Q9UI42 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15085-Q7RTY8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q9UI42-Q9Y5Y6 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|---------------|
| lpyt | P00747-P15085-Q8N4T0-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15085-Q86T26 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P48052-Q7RTY8 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8IVL8-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-Q8IVL8 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-Q8IVL8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q86T26-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | P00747-P05981-P15085-P48052 | 9606 | Homo sapiens |
| lpyt | B7Z1L4-P00747-P15085-P48052 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q86T26-Q8IVL8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7RTY8-Q9UI42 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7RTY8-Q8IVL8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15088-Q6UWY2 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7RTY8-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q86T26-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15085-Q9Y6M0 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-Q9UI42 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8N4T0-Q9Y6M0 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-P15085 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15085-Q7Z410 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-P48052 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7Z410-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | A8MTI9-P00747-P15085-P15088 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15088-Q04756 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q7Z410-Q9UI42 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q96IY4-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P48052-Q7Z410 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8IVL8-Q9Y6M0 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q86T26-Q9UI42 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15088-Q9UNI1 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8IU80-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P48052-Q86T26 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8IU80-Q9UI42 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15088-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P10323-P15085-Q8WXQ8 | 9606 | Homo sapiens |
| lpyt | P00747-P08217-P15085-P15088 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-P15086-Q9Y5Y6 | 9606 | Homo sapiens |
| lpyt | P00747-P10323-P15085-P15085 | 9606 | Homo sapiens |
| lpyt | P00747-P15085-Q8IU80-Q8N4T0 | 9606 | Homo sapiens |
| lpyt | B7Z459-P00747-P15085-Q8IVL8 | 9606 | Homo sapiens |
| lrew | Q3USS1-Q3USS1-Q3ZAS6-Q3ZAS6 | 10090 | Mus musculus |
| lrew | Q3USS1-Q3USS1-Q9WV56-Q9WV56 | 10090 | Mus musculus |
| lrew | O13107-O13107-O93243-O93243 | 7955 | Danio rerio |
| lrew | O13108-O13108-O93243-O93243 | 7955 | Danio rerio |
| lrew | O13107-O13107-Q66HY1-Q66HY1 | 7955 | Danio rerio |
| lrew | O13108-O13108-Q66HY1-Q66HY1 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-O13107-O13107 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-O13108-O13108 | 7955 | Danio rerio |
| lrew | A8E7N9-A8E7N9-O93243-O93243 | 7955 | Danio rerio |
| lrew | O93243-O93243-P85857-P85857 | 7955 | Danio rerio |
| lrew | O93243-O93243-Q0VG66-Q0VG66 | 7955 | Danio rerio |
| lrew | O93243-O93243-P35621-P35621 | 7955 | Danio rerio |
| lrew | Q0VG66-Q0VG66-Q66HY1-Q66HY1 | 7955 | Danio rerio |
| lrew | A8E7N9-A8E7N9-Q66HY1-Q66HY1 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-Q0VG66-Q0VG66 | 7955 | Danio rerio |
| lrew | A8E7N9-A8E7N9-C0L3D6-C0L3D6 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-P85857-P85857 | 7955 | Danio rerio |
| lrew | O13108-O13108-Q9W629-Q9W629 | 7955 | Danio rerio |
| lrew | O13107-O13107-Q9W629-Q9W629 | 7955 | Danio rerio |
| lrew | A8E7N9-A8E7N9-Q9W629-Q9W629 | 7955 | Danio rerio |
| lrew | O93243-O93243-Q7ZZT5-Q7ZZT5 | 7955 | Danio rerio |
| lrew | O93243-O93243-P87358-P87358 | 7955 | Danio rerio |
| lrew | O13144-O13144-Q66HY1-Q66HY1 | 7955 | Danio rerio |
| lrew | O13144-O13144-O93243-O93243 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-Q7ZZT5-Q7ZZT5 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-P87358-P87358 | 7955 | Danio rerio |
| lrew | C0L3D6-C0L3D6-O13144-O13144 | 7955 | Danio rerio |
| lrew | O13144-O13144-Q9W629-Q9W629 | 7955 | Danio rerio |
| lrew | Q90752-Q90752-Q90754-Q90754 | 9031 | Gallus gallus |
| lrew | Q90754-Q90754-Q9I8T6-Q9I8T6 | 9031 | Gallus gallus |
| lrew | Q90754-Q90754-Q9W6G0-Q9W6G0 | 9031 | Gallus gallus |
| lrew | P34822-P34822-Q90754-Q90754 | 9031 | Gallus gallus |
| lrew | Q90754-Q90754-Q9PVK1-Q9PVK1 | 9031 | Gallus gallus |
| lrew | Q90754-Q90754-Q9YHW9-Q9YHW9 | 9031 | Gallus gallus |
| lrew | B1AKZ9-B1AKZ9-P36894-P36894 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|------------------------|
| lrew | O95972-O95972-P36894-P36894 | 9606 | Homo sapiens |
| lrew | A5PJI9-A5PJI9-Q06AL7-Q06AL7 | 9913 | Bos taurus |
| lrew | P55106-P55106-Q06AL7-Q06AL7 | 9913 | Bos taurus |
| lrew | Q4TFB9-Q4TFB9-Q804S2-Q804S2 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RGZ0-Q4RGZ0-Q804S2-Q804S2 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RGZ0-Q4RGZ0-Q4RMK1-Q4RMK1 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RMK1-Q4RMK1-Q4TFB9-Q4TFB9 | 99883 | Tetraodon nigroviridis |
| lrew | Q4SJF6-Q4SJF6-Q804S2-Q804S2 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RMK1-Q4RMK1-Q4SJF6-Q4SJF6 | 99883 | Tetraodon nigroviridis |
| lrew | Q4SZ19-Q4SZ19-Q4TFB9-Q4TFB9 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RGZ0-Q4RGZ0-Q4SZ19-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| lrew | Q4RGZ0-Q4RGZ0-Q4T2Q4-Q4T2Q4 | 99883 | Tetraodon nigroviridis |
| lrew | Q4T2Q4-Q4T2Q4-Q4TFB9-Q4TFB9 | 99883 | Tetraodon nigroviridis |
| lrew | Q4SJF6-Q4SJF6-Q4SZ19-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| lrew | Q4SJF6-Q4SJF6-Q4T2Q4-Q4T2Q4 | 99883 | Tetraodon nigroviridis |
| ls4y | P18331-P18331-P38445-P38445 | 10116 | Rattus norvegicus |
| ls4y | P17491-P17491-P38445-P38445 | 10116 | Rattus norvegicus |
| ls4y | P17491-P17491-P38444-P38444 | 10116 | Rattus norvegicus |
| ls4y | P38445-P38445-Q9Z217-Q9Z217 | 10116 | Rattus norvegicus |
| ls4y | P38445-P38445-Q6HA10-Q6HA10 | 10116 | Rattus norvegicus |
| ls4y | P38444-P38444-Q6HA10-Q6HA10 | 10116 | Rattus norvegicus |
| ls4y | P38444-P38444-Q9Z217-Q9Z217 | 10116 | Rattus norvegicus |
| ls4y | P38445-P38445-P49002-P49002 | 10116 | Rattus norvegicus |
| ls4y | P38445-P38445-P55108-P55108 | 10116 | Rattus norvegicus |
| ls4y | P38444-P38444-P49002-P49002 | 10116 | Rattus norvegicus |
| ls4y | P38444-P38444-P55108-P55108 | 10116 | Rattus norvegicus |
| ls4y | Q4V965-Q4V965-Q8QGE3-Q8QGE3 | 7955 | Danio rerio |
| ls4y | AlL1T8-AlL1T8-Q4V965-Q4V965 | 7955 | Danio rerio |
| ls4y | AlL1T8-AlL1T8-A9CAY0-A9CAY0 | 7955 | Danio rerio |
| ls4y | B0S7E0-B0S7E0-Q4V965-Q4V965 | 7955 | Danio rerio |
| ls4y | A9CAY0-A9CAY0-B0S7E0-B0S7E0 | 7955 | Danio rerio |
| ls4y | P85857-P85857-Q4V965-Q4V965 | 7955 | Danio rerio |
| ls4y | P87358-P87358-Q4V965-Q4V965 | 7955 | Danio rerio |
| ls4y | Q13107-Q13107-Q4V965-Q4V965 | 7955 | Danio rerio |
| ls4y | A9CAY0-A9CAY0-Q13107-Q13107 | 7955 | Danio rerio |
| ls4y | O42220-O42220-Q90670-Q90670 | 9031 | Gallus gallus |
| ls4y | O42220-O42220-Q90669-Q90669 | 9031 | Gallus gallus |
| ls4y | Q90670-Q90670-Q9W6G0-Q9W6G0 | 9031 | Gallus gallus |
| ls4y | Q90669-Q90669-Q9W6G0-Q9W6G0 | 9031 | Gallus gallus |
| ls4y | Q90670-Q90670-Q90752-Q90752 | 9031 | Gallus gallus |
| ls4y | Q90670-Q90670-Q9I8T6-Q9I8T6 | 9031 | Gallus gallus |
| ls4y | Q90669-Q90669-Q90752-Q90752 | 9031 | Gallus gallus |
| ls4y | Q90669-Q90669-Q9I8T6-Q9I8T6 | 9031 | Gallus gallus |
| ls4y | P34822-P34822-Q90670-Q90670 | 9031 | Gallus gallus |
| ls4y | P34822-P34822-Q90669-Q90669 | 9031 | Gallus gallus |
| ls4y | B1AKZ9-B1AKZ9-Q13705-Q13705 | 9606 | Homo sapiens |
| ls4y | B1AKZ9-B1AKZ9-P27037-P27037 | 9606 | Homo sapiens |
| ls4y | O18836-O18836-Q95126-Q95126 | 9913 | Bos taurus |
| ls4y | O18836-O18836-Q28043-Q28043 | 9913 | Bos taurus |
| ls4y | P55106-P55106-Q95126-Q95126 | 9913 | Bos taurus |
| ls4y | P55106-P55106-Q28043-Q28043 | 9913 | Bos taurus |
| ls4y | P22444-P22444-Q95126-Q95126 | 9913 | Bos taurus |
| ls4y | P22444-P22444-Q28043-Q28043 | 9913 | Bos taurus |
| ls4y | Q2KJH1-Q2KJH1-Q95126-Q95126 | 9913 | Bos taurus |
| ls4y | A5PJI9-A5PJI9-Q95126-Q95126 | 9913 | Bos taurus |
| ls4y | Q28043-Q28043-Q2KJH1-Q2KJH1 | 9913 | Bos taurus |
| ls4y | A5PJI9-A5PJI9-Q28043-Q28043 | 9913 | Bos taurus |
| ls4y | Q4RWT9-Q4RWT9-Q4S1Z3-Q4S1Z3 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RWT9-Q4RWT9-Q4SES4-Q4SES4 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMV4-Q4RMV4-Q4S1Z3-Q4S1Z3 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMV4-Q4RMV4-Q4SES4-Q4SES4 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RWT9-Q4RWT9-Q4SZ19-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMV4-Q4RMV4-Q4SZ19-Q4SZ19 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RWT9-Q4RWT9-Q804S2-Q804S2 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMK1-Q4RMK1-Q4RWT9-Q4RWT9 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMV4-Q4RMV4-Q804S2-Q804S2 | 99883 | Tetraodon nigroviridis |
| ls4y | Q4RMK1-Q4RMK1-Q4RMV4-Q4RMV4 | 99883 | Tetraodon nigroviridis |
| lsdd | Q7TN96-Q920H8 | 10116 | Rattus norvegicus |
| lstf | Q62426-Q80UB0 | 10090 | Mus musculus |
| lstf | P01041-P15242 | 10116 | Rattus norvegicus |
| lt0p | P21941-P32942 | 9606 | Homo sapiens |
| ltaw | O88301-Q61482 | 10090 | Mus musculus |
| ltaw | O88301-Q60709 | 10090 | Mus musculus |
| ltaw | Q61482-Q91Y82 | 10090 | Mus musculus |
| ltaw | Q60709-Q91Y82 | 10090 | Mus musculus |
| ltaw | P21845-Q61482 | 10090 | Mus musculus |
| ltaw | P21845-Q60709 | 10090 | Mus musculus |
| ltaw | Q60709-Q8K0D2 | 10090 | Mus musculus |
| ltaw | Q61482-Q8K0D2 | 10090 | Mus musculus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-------------------|----------------|-------------------|
| 1taw | Q61482-Q8VIF2 | 10090 | Mus musculus |
| 1taw | Q60709-Q8VIF2 | 10090 | Mus musculus |
| 1taw | Q60709-Q9QYN3 | 10090 | Mus musculus |
| 1taw | Q61482-Q9QYN3 | 10090 | Mus musculus |
| 1taw | Q61482-Q7M761 | 10090 | Mus musculus |
| 1taw | Q60709-Q7M761 | 10090 | Mus musculus |
| 1taw | Q61482-Q9R098 | 10090 | Mus musculus |
| 1taw | Q60709-Q9R098 | 10090 | Mus musculus |
| 1taw | Q61482-Q80WM7 | 10090 | Mus musculus |
| 1taw | Q60709-Q80WM7 | 10090 | Mus musculus |
| 1taw | Q14B25-Q60709 | 10090 | Mus musculus |
| 1taw | Q14B25-Q61482 | 10090 | Mus musculus |
| 1taw | Q60709-Q91VE3 | 10090 | Mus musculus |
| 1taw | Q61482-Q91VE3 | 10090 | Mus musculus |
| 1taw | Q60709-Q99MS4 | 10090 | Mus musculus |
| 1taw | Q61482-Q99MS4 | 10090 | Mus musculus |
| 1taw | Q5K2P8-Q61482 | 10090 | Mus musculus |
| 1taw | Q5K2P8-Q60709 | 10090 | Mus musculus |
| 1taw | Q61482-Q61759 | 10090 | Mus musculus |
| 1taw | Q60709-Q61759 | 10090 | Mus musculus |
| 1taw | Q60709-Q8BJR6 | 10090 | Mus musculus |
| 1taw | Q61482-Q8BJR6 | 10090 | Mus musculus |
| 1taw | Q3UKY7-Q60709 | 10090 | Mus musculus |
| 1taw | Q3UKY7-Q61482 | 10090 | Mus musculus |
| 1taw | Q571E5-Q60709 | 10090 | Mus musculus |
| 1taw | Q571E5-Q61482 | 10090 | Mus musculus |
| 1taw | P05208-Q61482 | 10090 | Mus musculus |
| 1taw | P05208-Q60709 | 10090 | Mus musculus |
| 1taw | Q14B24-Q60709 | 10090 | Mus musculus |
| 1taw | Q14B24-Q61482 | 10090 | Mus musculus |
| 1taw | Q61482-Q9D9G7 | 10090 | Mus musculus |
| 1taw | Q60709-Q9D9G7 | 10090 | Mus musculus |
| 1taw | Q61482-Q8K4I7 | 10090 | Mus musculus |
| 1taw | Q60709-Q8K4I7 | 10090 | Mus musculus |
| 1taw | P43430-Q61482 | 10090 | Mus musculus |
| 1taw | P43430-Q60709 | 10090 | Mus musculus |
| 1taw | Q61482-Q8BW11 | 10090 | Mus musculus |
| 1taw | Q60709-Q8BW11 | 10090 | Mus musculus |
| 1taw | Q61482-Q9DAA4 | 10090 | Mus musculus |
| 1taw | P08426-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P00762-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P00763-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P27435-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P50343-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6L711-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q5M879-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P32822-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P32821-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q5EBA7-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q5K2P9-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P00773-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P16296-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P12788-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P18292-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P31394-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q5FVS2-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6BEA2-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P00774-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P09650-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P97594-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6IE59-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6IE62-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P50339-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | P97592-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6IE06-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1taw | Q6P6Q5-Q6TUF8 | 10116 | Rattus norvegicus |
| 1taw | P07477-Q06481 | 9606 | Homo sapiens |
| 1taw | P20231-Q06481 | 9606 | Homo sapiens |
| 1taw | Q06481-Q15661 | 9606 | Homo sapiens |
| 1taw | P40313-Q06481 | 9606 | Homo sapiens |
| 1taw | Q06481-Q8NHM4 | 9606 | Homo sapiens |
| 1taw | P35030-Q06481 | 9606 | Homo sapiens |
| 1taw | Q06481-Q9UBX7 | 9606 | Homo sapiens |
| 1taw | Q06481-Q14520 | 9606 | Homo sapiens |
| 1taw | P08519-Q06481 | 9606 | Homo sapiens |
| 1taw | Q06481-Q7RTY7 | 9606 | Homo sapiens |
| 1taw | Q06481-Q7Z5A4 | 9606 | Homo sapiens |
| 1taw | Q06481-Q7RTZ1 | 9606 | Homo sapiens |
| 1taw | B4DN26-Q06481 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates | | Taxonomy | |
|------------|-----------------------------|----------|--------------|
| (PDB code) | Protein complexes | ID | Species |
| ltaw | B4DNJ1-Q06481 | 9606 | Homo sapiens |
| ltaw | B4DV92-Q06481 | 9606 | Homo sapiens |
| ltaw | P00750-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q8NF86 | 9606 | Homo sapiens |
| ltaw | O43240-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q9UKQ9 | 9606 | Homo sapiens |
| ltaw | Q04756-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q9H2R5 | 9606 | Homo sapiens |
| ltaw | Q06481-Q9UNI1 | 9606 | Homo sapiens |
| ltaw | P15157-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q7RTY5 | 9606 | Homo sapiens |
| ltaw | P17538-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q6GPI1 | 9606 | Homo sapiens |
| ltaw | P49862-Q06481 | 9606 | Homo sapiens |
| ltaw | A6NIE9-Q06481 | 9606 | Homo sapiens |
| ltaw | B4DPQ7-Q06481 | 9606 | Homo sapiens |
| ltaw | Q06481-Q9Y5K2 | 9606 | Homo sapiens |
| ltaw | P08217-Q06481 | 9606 | Homo sapiens |
| ltco | P48454-P63098-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-P62942-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-Q5VVH2-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-P68106-Q6PIL6 | 9606 | Homo sapiens |
| ltco | O95302-P48454-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-Q00688-Q6PIL6 | 9606 | Homo sapiens |
| ltco | O95302-P48454-Q96PH1 | 9606 | Homo sapiens |
| ltco | P26885-P48454-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-Q6PIL6-Q96AY3 | 9606 | Homo sapiens |
| ltco | P48454-Q02790-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-Q00688-Q96PH1 | 9606 | Homo sapiens |
| ltco | P26885-P48454-Q96PH1 | 9606 | Homo sapiens |
| ltco | P48454-Q96AY3-Q96PH1 | 9606 | Homo sapiens |
| ltco | P48454-Q02790-Q96PH1 | 9606 | Homo sapiens |
| ltco | P48454-Q6PIL6-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-Q9NYL4-Q9UM19 | 9606 | Homo sapiens |
| ltco | P48454-Q99828-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-Q13451-Q6PIL6 | 9606 | Homo sapiens |
| ltco | P48454-Q96PH1-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-P61601-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-Q13451-Q96PH1 | 9606 | Homo sapiens |
| ltco | P48454-P62158-Q9NYL4 | 9606 | Homo sapiens |
| ltco | P48454-Q6PIL6-Q9NWM8 | 9606 | Homo sapiens |
| ltco | P48454-Q96PH1-Q9NWM8 | 9606 | Homo sapiens |
| ltfx | A2ARA0-A2ARA0-Q14BX2-Q14BX2 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q14BX2-Q14BX2 | 10090 | Mus musculus |
| ltfx | Q14BX2-Q14BX2-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q8VCA5-Q8VCA5 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q8VCA5-Q8VCA5 | 10090 | Mus musculus |
| ltfx | Q8BSB7-Q8BSB7-Q8VCA5-Q8VCA5 | 10090 | Mus musculus |
| ltfx | Q8BSB7-Q8BSB7-Q9ER04-Q9ER04 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q9ER04-Q9ER04 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q9ER04-Q9ER04 | 10090 | Mus musculus |
| ltfx | Q8BSB7-Q8BSB7-Q9D9M0-Q9D9M0 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q9D9M0-Q9D9M0 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q9D9M0-Q9D9M0 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q9QYZ9-Q9QYZ9 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q9QYZ9-Q9QYZ9 | 10090 | Mus musculus |
| ltfx | Q8BSB7-Q8BSB7-Q9QYZ9-Q9QYZ9 | 10090 | Mus musculus |
| ltfx | Q3UKE3-Q3UKE3-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q3UKE3-Q3UKE3 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q3UKE3-Q3UKE3 | 10090 | Mus musculus |
| ltfx | Q812A6-Q812A6-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q812A6-Q812A6 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q812A6-Q812A6 | 10090 | Mus musculus |
| ltfx | Q3TZ06-Q3TZ06-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q3TZ06-Q3TZ06 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q3TZ06-Q3TZ06 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q9QUL7-Q9QUL7 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q9QUL7-Q9QUL7 | 10090 | Mus musculus |
| ltfx | Q8BSB7-Q8BSB7-Q9QUL7-Q9QUL7 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q5U405-Q5U405 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q5U405-Q5U405 | 10090 | Mus musculus |
| ltfx | Q5U405-Q5U405-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-Q8BIK6-Q8BIK6 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-Q8BIK6-Q8BIK6 | 10090 | Mus musculus |
| ltfx | Q8BIK6-Q8BIK6-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | P97435-P97435-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| ltfx | A2ARA3-A2ARA3-P97435-P97435 | 10090 | Mus musculus |
| ltfx | A2ARA0-A2ARA0-P97435-P97435 | 10090 | Mus musculus |
| ltfx | Q80X17-Q80X17-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|----------------------|
| 1tfx | A2ARA3-A2ARA3-Q80X17-Q80X17 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q80X17-Q80X17 | 10090 | Mus musculus |
| 1tfx | Q8BSB7-Q8BSB7-Q920S2-Q920S2 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-Q920S2-Q920S2 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q920S2-Q920S2 | 10090 | Mus musculus |
| 1tfx | B2RWX8-B2RWX8-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-B2RWX8-B2RWX8 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-B2RWX8-B2RWX8 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q9Z319-Q9Z319 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-Q9Z319-Q9Z319 | 10090 | Mus musculus |
| 1tfx | Q8BSB7-Q8BSB7-Q9Z319-Q9Z319 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q566K6-Q566K6 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-Q566K6-Q566K6 | 10090 | Mus musculus |
| 1tfx | Q566K6-Q566K6-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| 1tfx | B2RRC6-B2RRC6-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-B2RRC6-B2RRC6 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-B2RRC6-B2RRC6 | 10090 | Mus musculus |
| 1tfx | Q3V0Q7-Q3V0Q7-Q8BSB7-Q8BSB7 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-Q3V0Q7-Q3V0Q7 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q3V0Q7-Q3V0Q7 | 10090 | Mus musculus |
| 1tfx | A2ARA0-A2ARA0-Q9JHJ7-Q9JHJ7 | 10090 | Mus musculus |
| 1tfx | A2ARA3-A2ARA3-Q9JHJ7-Q9JHJ7 | 10090 | Mus musculus |
| 1tfx | Q8BSB7-Q8BSB7-Q9JHJ7-Q9JHJ7 | 10090 | Mus musculus |
| 1tfx | P83748-P83748-Q5PQU8-Q5PQU8 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q8CJ17-Q8CJ17 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q8CJ16-Q8CJ16 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q6P7D7-Q6P7D7 | 10116 | Rattus norvegicus |
| 1tfx | B2RYJ5-B2RYJ5-Q5PQU8-Q5PQU8 | 10116 | Rattus norvegicus |
| 1tfx | P86091-P86091-Q5PQU8-Q5PQU8 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q80YN4-Q80YN4 | 10116 | Rattus norvegicus |
| 1tfx | P69526-P69526-Q5PQU8-Q5PQU8 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q6IE07-Q6IE07 | 10116 | Rattus norvegicus |
| 1tfx | Q5PQU8-Q5PQU8-Q9Z1D3-Q9Z1D3 | 10116 | Rattus norvegicus |
| 1tfx | P10323-P10323-P10646-P10646 | 9606 | Homo sapiens |
| 1tfx | A7E330-A7E330-Q1LZ77-Q1LZ77 | 9913 | Bos taurus |
| 1tfx | A6QPX2-A6QPX2-Q1LZ77-Q1LZ77 | 9913 | Bos taurus |
| 1tfx | Q0IIH7-Q0IIH7-Q1LZ77-Q1LZ77 | 9913 | Bos taurus |
| 1tfx | A2VDV7-A2VDV7-Q1LZ77-Q1LZ77 | 9913 | Bos taurus |
| 1tfx | P98072-P98072-Q1LZ77-Q1LZ77 | 9913 | Bos taurus |
| 1tfx | Q1LZ77-Q1LZ77-Q32PI4-Q32PI4 | 9913 | Bos taurus |
| 1tfx | Q1LZ77-Q1LZ77-Q2YDL8-Q2YDL8 | 9913 | Bos taurus |
| luad | O54921-O54921-P63033-P63033 | 10116 | Rattus norvegicus |
| luea | P07152-P07152-P48032-P48032 | 10116 | Rattus norvegicus |
| luea | P48032-P48032-P50280-P50280 | 10116 | Rattus norvegicus |
| luea | P48032-P48032-Q499S5-Q499S5 | 10116 | Rattus norvegicus |
| luea | A1EC81-A1EC81-P48032-P48032 | 10116 | Rattus norvegicus |
| luea | C0M4B0-C0M4B0-P48032-P48032 | 10116 | Rattus norvegicus |
| luea | B5DFD5-B5DFD5-P48032-P48032 | 10116 | Rattus norvegicus |
| luea | O88272-O88272-P48032-P48032 | 10116 | Rattus norvegicus |
| lukv | P37727-P51158 | 10116 | Rattus norvegicus |
| lvgo | A2AD03-Q99KL7 | 10090 | Mus musculus |
| lvgo | Q99KL7-Q9QXG2 | 10090 | Mus musculus |
| lvgo | Q99KL7-Q9QZD5 | 10090 | Mus musculus |
| lvgo | P37727-P51158 | 10116 | Rattus norvegicus |
| lvgo | P24386-P51157 | 9606 | Homo sapiens |
| lvgo | P26374-P51157 | 9606 | Homo sapiens |
| lw98 | B1WC54-Q5U2X5 | 10116 | Rattus norvegicus |
| lw98 | P39949-Q5U2X5 | 10116 | Rattus norvegicus |
| lw98 | B1WC54-Q2PYT3 | 10116 | Rattus norvegicus |
| lw98 | Q5U2X5-Q6AY13 | 10116 | Rattus norvegicus |
| lw98 | Q2PYT3-Q6AY13 | 10116 | Rattus norvegicus |
| lw98 | Q5U2X5-Q6GX89 | 10116 | Rattus norvegicus |
| lw98 | P30277-Q5U2X5 | 10116 | Rattus norvegicus |
| lw98 | Q5M857-Q5U2X5 | 10116 | Rattus norvegicus |
| lw98 | Q2PYT3-Q5M857 | 10116 | Rattus norvegicus |
| lw98 | Q8LPH3-Q9C6Y3 | 3702 | Arabidopsis thaliana |
| lw98 | Q9C6Y3-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| lw98 | Q39069-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q9C6Y3-Q9LSM7 | 3702 | Arabidopsis thaliana |
| lw98 | Q8LPH3-Q9C968 | 3702 | Arabidopsis thaliana |
| lw98 | P30183-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q8LPH3-Q9LDM4 | 3702 | Arabidopsis thaliana |
| lw98 | O48790-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q147G5-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q39068-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q39069-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| lw98 | Q38818-Q8LPH3 | 3702 | Arabidopsis thaliana |
| lw98 | Q9C6Y3-Q9LNN0 | 3702 | Arabidopsis thaliana |
| lw98 | Q3ECW2-Q8LPH3 | 3702 | Arabidopsis thaliana |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|---|----------------|-----------------------------|
| 1w98 | Q39067-Q8LPH3 | 3702 | Arabidopsis thaliana |
| 1w98 | A0MEB5-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | Q38818-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | Q39069-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q147G5-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | P30183-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9C968-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | A0MEB5-Q8LPH3 | 3702 | Arabidopsis thaliana |
| 1w98 | Q39070-Q8LPH3 | 3702 | Arabidopsis thaliana |
| 1w98 | Q3ECW2-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | Q147G5-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9LDM4-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | A0MEB5-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q3ECW2-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q38818-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9C6Y3-Q9FKV9 | 3702 | Arabidopsis thaliana |
| 1w98 | P30183-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9C968-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9LDM4-Q9LSM7 | 3702 | Arabidopsis thaliana |
| 1w98 | Q9SA32-Q9ZVM9 | 3702 | Arabidopsis thaliana |
| 1w98 | P53682-Q0JNK6 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q7F830 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q0JPA4 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q2QN26 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q2QQ96 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q0D9C7 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q0DJR9 | 39947 | Oryza sativa Japonica Group |
| 1w98 | P53682-Q7I5I4 | 39947 | Oryza sativa Japonica Group |
| 1w98 | B7Z7E3-Q8TD08 | 9606 | Homo sapiens |
| 1w98 | P78396-Q8TD08 | 9606 | Homo sapiens |
| 1w98 | Q17R13-Q5E9K7 | 9913 | Bos taurus |
| 1w98 | Q17R13-Q1LZG6 | 9913 | Bos taurus |
| 1w98 | O77689-Q17R13 | 9913 | Bos taurus |
| 1w98 | Q0P5D3-Q17R13 | 9913 | Bos taurus |
| 1wa5 | P52293-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | O35345-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | P63032-Q4FJZ2-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | P63032-Q60960-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | O35344-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | C0LLJ0-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | C0LLJ1-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | P63032-Q58HC5-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | O35343-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | P63032-Q9CT07-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | A6PW68-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | A2A601-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1wa5 | A2A600-P63032-Q9ERK4 | 10090 | Mus musculus |
| 1xhm | Q61016-Q8C7V3 | 10090 | Mus musculus |
| 1xhm | P50153-Q8C7V3 | 10090 | Mus musculus |
| 1xhm | Q8C7V3-Q9DAS9 | 10090 | Mus musculus |
| 1xhm | P63216-Q8C7V3 | 10090 | Mus musculus |
| 1xhm | P63078-Q8C7V3 | 10090 | Mus musculus |
| 1xhm | A2RRU3-P43425 | 10116 | Rattus norvegicus |
| 1xhm | A2RRU3-O35356 | 10116 | Rattus norvegicus |
| 1xhm | A2RRU3-P63077 | 10116 | Rattus norvegicus |
| 1xhm | Q5F3D7-Q5ZJ48 | 9031 | Gallus gallus |
| 1xhm | O60262-Q8TED0 | 9606 | Homo sapiens |
| 1xhm | P50150-Q8TED0 | 9606 | Homo sapiens |
| 1xhm | Q8TED0-Q9UK08 | 9606 | Homo sapiens |
| 1xhm | A7MB12-Q28024 | 9913 | Bos taurus |
| 1xhm | A4IFL6-A7MB12 | 9913 | Bos taurus |
| 1xhm | A7MB12-P30671 | 9913 | Bos taurus |
| 1xhm | A7MB12-P63214 | 9913 | Bos taurus |
| 1xhm | Q4RMR9-Q4RUV7 | 99883 | Tetraodon nigroviridis |
| 1xhm | Q4REG3-Q4RUV7 | 99883 | Tetraodon nigroviridis |
| 1xhm | Q4RUV7-Q4SFP0 | 99883 | Tetraodon nigroviridis |
| 1xhm | Q4RUV7-Q4SCQ2 | 99883 | Tetraodon nigroviridis |
| 1xwd | P04652-P04652-P20395-P20395-Q6P509-Q6P509 | 10116 | Rattus norvegicus |
| 1xwd | P79763-P79763-Q6T5C1-Q6T5C1-Q8QGF8-Q8QGF8 | 9031 | Gallus gallus |
| 1xwd | Q6T5C1-Q6T5C1-Q76N37-Q76N37-Q8QGF8-Q8QGF8 | 9031 | Gallus gallus |
| 1xwd | P01215-P01215-P01222-P01222-P23945-P23945 | 9606 | Homo sapiens |
| 1xwd | P01215-P01215-P23945-P23945-Q15962-Q15962 | 9606 | Homo sapiens |
| 1xwd | P01215-P01215-Q05AH0-Q05AH0-Q15962-Q15962 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| 1ya5 | O70548-Q3UQ28-Q3UQ28 | 10090 | Mus musculus |
| 1yc0 | Q9ER04-Q9R097 | 10090 | Mus musculus |
| 1yc0 | B2RY54-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q8VCA5-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q5U405-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9DBI0-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q14BX2-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q3UKE3-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9D9M0-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9QUL7-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9QYZ9-Q9R097 | 10090 | Mus musculus |
| 1yc0 | P97435-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q3TZ06-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q812A6-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q80X17-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q8BIK6-Q9R097 | 10090 | Mus musculus |
| 1yc0 | B2RWX8-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q920S2-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9JHJ7-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q566K6-Q9R097 | 10090 | Mus musculus |
| 1yc0 | B2RRC6-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q9R097-Q9Z319 | 10090 | Mus musculus |
| 1yc0 | Q3V0Q7-Q9R097 | 10090 | Mus musculus |
| 1yc0 | P21812-Q9R097 | 10090 | Mus musculus |
| 1yc0 | Q3UN88-Q9R097 | 10090 | Mus musculus |
| 1yc0 | P28293-Q9R097 | 10090 | Mus musculus |
| 1yc0 | P15119-Q9R097 | 10090 | Mus musculus |
| 1yc0 | A4QPC5-Q9R097 | 10090 | Mus musculus |
| 1yc0 | O35164-Q9R097 | 10090 | Mus musculus |
| 1yc0 | B7ZNH6-Q9R097 | 10090 | Mus musculus |
| 1yc0 | B4DV92-O43291 | 9606 | Homo sapiens |
| 1yc0 | B4DN26-O43291 | 9606 | Homo sapiens |
| 1yc0 | B4DNJ1-O43291 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q8NF86 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q7RTY7 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9UBX7 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q15661 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q7Z5A4 | 9606 | Homo sapiens |
| 1yc0 | O43291-P20231 | 9606 | Homo sapiens |
| 1yc0 | O43291-P08519 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q7RTZ1 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9UKQ9 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9UNI1 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9H2R5 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9BQR3 | 9606 | Homo sapiens |
| 1yc0 | B4DPQ3-O43291 | 9606 | Homo sapiens |
| 1yc0 | B4DPQ7-O43291 | 9606 | Homo sapiens |
| 1yc0 | A6NIE9-O43291 | 9606 | Homo sapiens |
| 1yc0 | O00187-O43291 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q7RTY5 | 9606 | Homo sapiens |
| 1yc0 | A1L453-O43291 | 9606 | Homo sapiens |
| 1yc0 | O43291-P15157 | 9606 | Homo sapiens |
| 1yc0 | O43291-P09871 | 9606 | Homo sapiens |
| 1yc0 | O43291-P49863 | 9606 | Homo sapiens |
| 1yc0 | O43291-P49862 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9GZN4 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9Y5K2 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q9BZJ3 | 9606 | Homo sapiens |
| 1yc0 | A8MTI9-O43291 | 9606 | Homo sapiens |
| 1yc0 | O43291-P08217 | 9606 | Homo sapiens |
| 1yc0 | O43291-P07288 | 9606 | Homo sapiens |
| 1yc0 | O43291-P23946 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q6UWY2 | 9606 | Homo sapiens |
| 1yc0 | O43291-P08861 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q8IYP2 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q2L4Q9 | 9606 | Homo sapiens |
| 1yc0 | O43291-P08218 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q2TV78 | 9606 | Homo sapiens |
| 1yc0 | O43291-Q15096 | 9606 | Homo sapiens |
| 1yc0 | O43291-P26927 | 9606 | Homo sapiens |
| 1yc0 | B4DMX2-O43291 | 9606 | Homo sapiens |
| 1yph | P28293-P28293-Q99MS4-Q99MS4 | 10090 | Mus musculus |
| 1yph | P07146-P07146-P28293-P28293 | 10090 | Mus musculus |
| 1yph | P07338-P07338-Q6GQQ3-Q6GQQ3 | 10116 | Rattus norvegicus |
| 1z2c | A6NML8-A6NML8-P52198-P52198 | 9606 | Homo sapiens |
| 1z2c | A8MSQ4-A8MSQ4-P52198-P52198 | 9606 | Homo sapiens |
| 1z2c | O60879-O60879-P52198-P52198 | 9606 | Homo sapiens |
| 1zbd | P47708-Q8CFP6 | 10090 | Mus musculus |
| 1zbd | P47708-Q05D38 | 10090 | Mus musculus |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-------------------|----------------|-------------------|
| 1zjd | Q60709-Q8VIF2 | 10090 | Mus musculus |
| 1zjd | Q61482-Q8VIF2 | 10090 | Mus musculus |
| 1zjd | Q60709-Q9QYN3 | 10090 | Mus musculus |
| 1zjd | Q61482-Q9QYN3 | 10090 | Mus musculus |
| 1zjd | P21845-Q61482 | 10090 | Mus musculus |
| 1zjd | P21845-Q60709 | 10090 | Mus musculus |
| 1zjd | Q61482-Q91Y82 | 10090 | Mus musculus |
| 1zjd | Q60709-Q91Y82 | 10090 | Mus musculus |
| 1zjd | O88301-Q61482 | 10090 | Mus musculus |
| 1zjd | O88301-Q60709 | 10090 | Mus musculus |
| 1zjd | Q61482-Q9R098 | 10090 | Mus musculus |
| 1zjd | Q60709-Q9R098 | 10090 | Mus musculus |
| 1zjd | Q61482-Q7M761 | 10090 | Mus musculus |
| 1zjd | Q60709-Q7M761 | 10090 | Mus musculus |
| 1zjd | Q60709-Q80WM7 | 10090 | Mus musculus |
| 1zjd | Q61482-Q80WM7 | 10090 | Mus musculus |
| 1zjd | Q61482-Q8KOD2 | 10090 | Mus musculus |
| 1zjd | Q60709-Q8KOD2 | 10090 | Mus musculus |
| 1zjd | Q61482-Q99MS4 | 10090 | Mus musculus |
| 1zjd | Q60709-Q99MS4 | 10090 | Mus musculus |
| 1zjd | Q60709-Q91VE3 | 10090 | Mus musculus |
| 1zjd | Q5K2P8-Q60709 | 10090 | Mus musculus |
| 1zjd | Q5K2P8-Q61482 | 10090 | Mus musculus |
| 1zjd | Q61482-Q91VE3 | 10090 | Mus musculus |
| 1zjd | Q3UKY7-Q60709 | 10090 | Mus musculus |
| 1zjd | Q3UKY7-Q61482 | 10090 | Mus musculus |
| 1zjd | Q14B25-Q60709 | 10090 | Mus musculus |
| 1zjd | Q14B25-Q61482 | 10090 | Mus musculus |
| 1zjd | Q61482-Q61759 | 10090 | Mus musculus |
| 1zjd | Q60709-Q61759 | 10090 | Mus musculus |
| 1zjd | Q60709-Q8BJR6 | 10090 | Mus musculus |
| 1zjd | Q61482-Q8BJR6 | 10090 | Mus musculus |
| 1zjd | P05208-Q60709 | 10090 | Mus musculus |
| 1zjd | P05208-Q61482 | 10090 | Mus musculus |
| 1zjd | Q14B24-Q60709 | 10090 | Mus musculus |
| 1zjd | Q14B24-Q61482 | 10090 | Mus musculus |
| 1zjd | Q571E5-Q61482 | 10090 | Mus musculus |
| 1zjd | Q571E5-Q60709 | 10090 | Mus musculus |
| 1zjd | Q61482-Q8K4I7 | 10090 | Mus musculus |
| 1zjd | Q60709-Q8K4I7 | 10090 | Mus musculus |
| 1zjd | Q60709-Q8BW11 | 10090 | Mus musculus |
| 1zjd | Q61482-Q8BW11 | 10090 | Mus musculus |
| 1zjd | P43430-Q60709 | 10090 | Mus musculus |
| 1zjd | P43430-Q61482 | 10090 | Mus musculus |
| 1zjd | Q61482-Q61646 | 10090 | Mus musculus |
| 1zjd | Q60709-Q61646 | 10090 | Mus musculus |
| 1zjd | P27435-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P00762-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P50343-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P08426-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P00763-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P32822-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P32821-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q5M879-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6L711-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q5EBA7-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q5K2P9-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P00773-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P18292-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q5FVS2-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P31394-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P12788-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6BEA2-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P16296-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P00774-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6IE62-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P09650-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P97594-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | P97592-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6IE06-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6IE59-Q6P6Q5 | 10116 | Rattus norvegicus |
| 1zjd | Q6P6Q5-Q6TUF8 | 10116 | Rattus norvegicus |
| 1zjd | P20231-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q15661 | 9606 | Homo sapiens |
| 1zjd | P07477-Q06481 | 9606 | Homo sapiens |
| 1zjd | B4DV92-Q06481 | 9606 | Homo sapiens |
| 1zjd | B4DNJ1-Q06481 | 9606 | Homo sapiens |
| 1zjd | B4DN26-Q06481 | 9606 | Homo sapiens |
| 1zjd | P00750-Q06481 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| 1zjd | Q06481-Q9UBX7 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q7Z5A4 | 9606 | Homo sapiens |
| 1zjd | P40313-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q8NF86 | 9606 | Homo sapiens |
| 1zjd | P08519-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q8NHM4 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q14520 | 9606 | Homo sapiens |
| 1zjd | Q04756-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q7RTZ1 | 9606 | Homo sapiens |
| 1zjd | O43240-Q06481 | 9606 | Homo sapiens |
| 1zjd | P35030-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q7RTY7 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q9UKQ9 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q9UNI1 | 9606 | Homo sapiens |
| 1zjd | A6NIE9-Q06481 | 9606 | Homo sapiens |
| 1zjd | B4DPQ3-Q06481 | 9606 | Homo sapiens |
| 1zjd | B4DPQ7-Q06481 | 9606 | Homo sapiens |
| 1zjd | A1L453-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q9H2R5 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q9Y5K2 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q7RTY5 | 9606 | Homo sapiens |
| 1zjd | P49862-Q06481 | 9606 | Homo sapiens |
| 1zjd | P15157-Q06481 | 9606 | Homo sapiens |
| 1zjd | Q06481-Q9BQR3 | 9606 | Homo sapiens |
| 1zr0 | O35536-O35536-Q14BX2-Q14BX2 | 10090 | Mus musculus |
| 1zr0 | B2RY54-B2RY54-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q8VCA5-Q8VCA5 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9ER04-Q9ER04 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q5U405-Q5U405 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9D9M0-Q9D9M0 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q3TZ06-Q3TZ06 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q812A6-Q812A6 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-P97435-P97435 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9QYZ9-Q9QYZ9 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q3UKE3-Q3UKE3 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9QUL7-Q9QUL7 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-P15119-P15119 | 10090 | Mus musculus |
| 1zr0 | B2RWX8-B2RWX8-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9JHJ7-Q9JHJ7 | 10090 | Mus musculus |
| 1zr0 | B2RRC6-B2RRC6-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q566K6-Q566K6 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9Z319-Q9Z319 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q920S2-Q920S2 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q8BIK6-Q8BIK6 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q3V0Q7-Q3V0Q7 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q80X17-Q80X17 | 10090 | Mus musculus |
| 1zr0 | O35164-O35164-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q9D9G7-Q9D9G7 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-P21812-P21812 | 10090 | Mus musculus |
| 1zr0 | O35536-O35536-Q3UN88-Q3UN88 | 10090 | Mus musculus |
| 1zr0 | A4QPC5-A4QPC5-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | B7ZNH6-B7ZNH6-O35536-O35536 | 10090 | Mus musculus |
| 1zr0 | P69526-P69526-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | Q8CF99-Q8CF99-Q8CJ17-Q8CJ17 | 10116 | Rattus norvegicus |
| 1zr0 | Q8CF99-Q8CF99-Q8CJ16-Q8CJ16 | 10116 | Rattus norvegicus |
| 1zr0 | P83748-P83748-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | B2RYJ5-B2RYJ5-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | Q6P7D7-Q6P7D7-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | Q80YN4-Q80YN4-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | P86091-P86091-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | Q6IE07-Q6IE07-Q8CF99-Q8CF99 | 10116 | Rattus norvegicus |
| 1zr0 | Q8CF99-Q8CF99-Q9Z1D3-Q9Z1D3 | 10116 | Rattus norvegicus |
| 1zr0 | P48307-P48307-Q9NRS4-Q9NRS4 | 9606 | Homo sapiens |
| 1zr0 | A8MYM4-A8MYM4-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q7Z410-Q7Z410 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q9Y5Y6-Q9Y5Y6 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q1RMF8-Q1RMF8 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q9BYE2-Q9BYE2 | 9606 | Homo sapiens |
| 1zr0 | P10323-P10323-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q9H3S3-Q9H3S3 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q5USC7-Q5USC7 | 9606 | Homo sapiens |
| 1zr0 | B7Z459-B7Z459-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q86T26-Q86T26 | 9606 | Homo sapiens |
| 1zr0 | B7WPR2-B7WPR2-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | B4DTM9-B4DTM9-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-P98073-P98073 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q9NRR2-Q9NRR2 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q7RTY9-Q7RTY9 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q86WS5-Q86WS5 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|-------------------|
| 1zr0 | P48307-P48307-Q9Y6M0-Q9Y6M0 | 9606 | Homo sapiens |
| 1zr0 | B4DRF2-B4DRF2-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q7RTY8-Q7RTY8 | 9606 | Homo sapiens |
| 1zr0 | P48307-P48307-Q6UWB4-Q6UWB4 | 9606 | Homo sapiens |
| 1zr0 | B7Z311-B7Z311-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P10144-P10144-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | P20718-P20718-P48307-P48307 | 9606 | Homo sapiens |
| 1zr0 | A7E330-A7E330-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | A6QPX2-A6QPX2-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | Q0IIH7-Q0IIH7-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | A2VDV7-A2VDV7-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | P98072-P98072-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | Q32PI4-Q32PI4-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 1zr0 | Q2YDL8-Q2YDL8-Q7YRQ8-Q7YRQ8 | 9913 | Bos taurus |
| 2b5i | P17108-P26896-P26897-Q7TP53 | 10116 | Rattus norvegicus |
| 2b7d | P20352-P70375-P97435 | 10090 | Mus musculus |
| 2b7d | P20352-P70375-Q5S248 | 10090 | Mus musculus |
| 2b7d | B2RY54-P20352-P70375 | 10090 | Mus musculus |
| 2b7d | P16294-P20352-P97435 | 10090 | Mus musculus |
| 2b7d | P20352-P56677-P70375 | 10090 | Mus musculus |
| 2b7d | P20352-P70375-Q80UR4 | 10090 | Mus musculus |
| 2b7d | P20352-P97435-Q9CQW3 | 10090 | Mus musculus |
| 2b7d | P20352-P70375-Q8BIK6 | 10090 | Mus musculus |
| 2b7d | P20352-Q5S248-Q9CQW3 | 10090 | Mus musculus |
| 2b7d | B2RY54-P16294-P20352 | 10090 | Mus musculus |
| 2b7d | P16294-P20352-P56677 | 10090 | Mus musculus |
| 2b7d | P16294-P20352-Q8BIK6 | 10090 | Mus musculus |
| 2b7d | P20352-P56677-Q9CQW3 | 10090 | Mus musculus |
| 2b7d | P20352-Q8BIK6-Q9CQW3 | 10090 | Mus musculus |
| 2b7d | P42533-P69526-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | P69526-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | Q66HI4-Q6AXZ6-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | P42533-Q6AXZ6-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | P86091-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | P42533-P86091-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | P31394-P86091-Q66HI4 | 10116 | Rattus norvegicus |
| 2b7d | P31394-P42533-P86091 | 10116 | Rattus norvegicus |
| 2b7d | B1H253-P86091-Q66HI4 | 10116 | Rattus norvegicus |
| 2b7d | B1H253-P42533-P86091 | 10116 | Rattus norvegicus |
| 2b7d | P42533-Q5QSK2-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | Q5QSK2-Q66HI4-Q8K3U6 | 10116 | Rattus norvegicus |
| 2b7d | B1H253-P42533-Q5QSK2 | 10116 | Rattus norvegicus |
| 2b7d | B1H253-Q5QSK2-Q66HI4 | 10116 | Rattus norvegicus |
| 2b7d | P31394-P42533-Q5QSK2 | 10116 | Rattus norvegicus |
| 2b7d | P31394-Q5QSK2-Q66HI4 | 10116 | Rattus norvegicus |
| 2b7d | B0UY88-B8A5T3-Q504H3 | 7955 | Danio rerio |
| 2b7d | A4QP82-B0UY88-B8A5T3 | 7955 | Danio rerio |
| 2b7d | P08709-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P98073-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q7Z410-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q7Z410-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-P00749-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P00749-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q6ZMR5-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7Z459-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-O15393-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | O15393-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q86WH4-Q9NRS4 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q86WH4-Q9NRS4 | 9606 | Homo sapiens |
| 2b7d | A8MYM4-Q5JVE8-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B4DPQ7-Q7Z410-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P08709-Q7RTY7-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B4DPQ7-Q86WH4-Q9NRS4 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q7RTY7-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P00742-Q7RTY7-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q7RTY7-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q86WH4-Q9UL52 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q86WH4-Q9UL52 | 9606 | Homo sapiens |
| 2b7d | P08709-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B4DPQ7-Q86WH4-Q9UL52 | 9606 | Homo sapiens |
| 2b7d | P00742-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P00740-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P08709-Q86WH4-Q9P0G3 | 9606 | Homo sapiens |
| 2b7d | Q5JVE8-Q86WH4-Q9P0G3 | 9606 | Homo sapiens |
| 2b7d | B7ZBK1-Q86WH4-Q9P0G3 | 9606 | Homo sapiens |
| 2b7d | B4DPQ7-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P04070-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |

Table S3. Gold standard negative set (Continued)

| Templates (PDB code) | Protein complexes | Taxonomy ID | Species |
|-------------------------|-----------------------------|----------------|----------------------|
| 2b7d | P22891-Q7Z5A4-Q86WH4 | 9606 | Homo sapiens |
| 2b7d | P22457-P30931-P98072 | 9913 | Bos taurus |
| 2b7d | P22457-P30931-Q05589 | 9913 | Bos taurus |
| 2b7d | P00743-P30931-P98072 | 9913 | Bos taurus |
| 2b7d | P00745-P30931-P98072 | 9913 | Bos taurus |
| 2b7d | P00741-P30931-P98072 | 9913 | Bos taurus |
| 2b7d | P00743-P30931-Q05589 | 9913 | Bos taurus |
| 2b7d | P00745-P30931-Q05589 | 9913 | Bos taurus |
| 2b7d | P00741-P30931-Q05589 | 9913 | Bos taurus |
| 2bki | P25071-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | P25070-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SIQ7-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SK73-Q9SSF8 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SK73-Q9SRE6 | 3702 | Arabidopsis thaliana |
| 2bki | Q8RWL2-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q1PFH8-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9M9V8-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SK73-Q9ZV15 | 3702 | Arabidopsis thaliana |
| 2bki | Q9S9V0-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q42438-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q38873-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9C6P3-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | O49717-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SK73-Q9ZSA3 | 3702 | Arabidopsis thaliana |
| 2bki | Q9SK73-Q9ZSA2 | 3702 | Arabidopsis thaliana |
| 2bki | Q8W4I7-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bki | Q9M101-Q9SK73 | 3702 | Arabidopsis thaliana |
| 2bo9 | P70202-P70202-Q8R4H4-Q8R4H4 | 10090 | Mus musculus |
| 2bo9 | P70202-P70202-Q9JHH6-Q9JHH6 | 10090 | Mus musculus |
| 2bo9 | P70202-P70202-Q6P8K8-Q6P8K8 | 10090 | Mus musculus |
| 2bo9 | P70202-P70202-Q504N0-Q504N0 | 10090 | Mus musculus |
| 2bo9 | P70202-P70202-Q5U901-Q5U901 | 10090 | Mus musculus |
| 2bo9 | P49788-P49788-Q96IY4-Q96IY4 | 9606 | Homo sapiens |
| 2bo9 | P15085-P15085-P49788-P49788 | 9606 | Homo sapiens |
| 2bo9 | P49788-P49788-Q8WXQ8-Q8WXQ8 | 9606 | Homo sapiens |
| 2bo9 | P49788-P49788-Q9UI42-Q9UI42 | 9606 | Homo sapiens |
| 2bo9 | P15086-P15086-P49788-P49788 | 9606 | Homo sapiens |
| 2bo9 | P49788-P49788-Q8IVL8-Q8IVL8 | 9606 | Homo sapiens |
| 2bo9 | P48052-P48052-P49788-P49788 | 9606 | Homo sapiens |
| 2bo9 | P49788-P49788-Q8N4T0-Q8N4T0 | 9606 | Homo sapiens |
| 2d9q | A2A8Y3-P09920 | 10090 | Mus musculus |
| 2d9q | P09920-P40223 | 10090 | Mus musculus |
| 2d9q | P09920-Q14BI3 | 10090 | Mus musculus |
| 2d9q | P13854-Q5F3Y5 | 9031 | Gallus gallus |
| 2fdb | O88182-O88182-Q498D6-Q498D6 | 10116 | Rattus norvegicus |
| 2fdb | O88182-O88182-Q9JHX9-Q9JHX9 | 10116 | Rattus norvegicus |
| 2fdb | O88182-O88182-Q63827-Q63827 | 10116 | Rattus norvegicus |
| 2fdb | O88182-O88182-Q04589-Q04589 | 10116 | Rattus norvegicus |
| 2fdb | A4JYI8-A4JYI8-Q805B2-Q805B2 | 7955 | Danio rerio |
| 2fdb | A4QN31-A4QN31-Q805B2-Q805B2 | 7955 | Danio rerio |
| 2fdb | Q805B2-Q805B2-Q8AYP3-Q8AYP3 | 7955 | Danio rerio |
| 2fdb | A4QN31-A4QN31-Q6SJP8-Q6SJP8 | 7955 | Danio rerio |
| 2fdb | A4JYI8-A4JYI8-Q6SJP8-Q6SJP8 | 7955 | Danio rerio |
| 2fdb | Q6SJP8-Q6SJP8-Q8AYP3-Q8AYP3 | 7955 | Danio rerio |
| 2fdb | Q805B2-Q805B2-Q805B9-Q805B9 | 7955 | Danio rerio |
| 2fdb | Q6SJP8-Q6SJP8-Q805B9-Q805B9 | 7955 | Danio rerio |
| 2fdb | B4DVP5-B4DVP5-P55075-P55075 | 9606 | Homo sapiens |
| 2fdb | P55075-P55075-Q59F30-Q59F30 | 9606 | Homo sapiens |
| 2fdb | O76093-O76093-Q59F30-Q59F30 | 9606 | Homo sapiens |
| 2fdb | B4DVP5-B4DVP5-O76093-O76093 | 9606 | Homo sapiens |
| 2fdb | B4DVP5-B4DVP5-O60258-O60258 | 9606 | Homo sapiens |
| 2fdb | O60258-O60258-Q59F30-Q59F30 | 9606 | Homo sapiens |
| 2fdb | P31371-P31371-Q59F30-Q59F30 | 9606 | Homo sapiens |
| 2fdb | B4DVP5-B4DVP5-P31371-P31371 | 9606 | Homo sapiens |
| 2fdb | B4DVP5-B4DVP5-O43320-O43320 | 9606 | Homo sapiens |
| 2fdb | O43320-O43320-Q59F30-Q59F30 | 9606 | Homo sapiens |
| 2trc | P62880-Q61012-Q9QW08 | 10090 | Mus musculus |
| 2trc | P61953-P62880-Q9QW08 | 10090 | Mus musculus |
| 2trc | P62880-Q61017-Q9QW08 | 10090 | Mus musculus |