# ClusPro-DC: Dimer Classification by the Cluspro Server for Protein-Protein Docking

# Supplemental Information

**Content**

## Supplementary Results and Discussion

### Selecting the threshold T for discrimination between biological and crystallographic dimers

As described in the main text and shown in **Fig. 2c**, based on the receiver operating characteristic (ROC) curve $T$ = 33 appears to be a reasonable choice for the threshold number of hits to distinguish between crystallographic and biological dimers. In good agreement with this selection, at $N_{nn}$ = 33 the probability $P$ of being a biological dimer is between 0.48 and 0.52, depending on the level of smoothing of the probability curve, and we select $P$ = 0.5 as the probability threshold between crystallographic and biological dimers. The predicted probability values are not very sensitive to the changes in the training set. **Fig. S1** shows the fraction of biological dimers as a function of $N_{nn}$ and the smoothed probability curve, now based on unified training and difficult test set, thus including 345 rather than 209 proteins. The curve based on the training set (**Fig. 2b),** and the one based on the combination of training and difficult test sets **(Fig. S1)** are very similar, and the probability $P$ of being biological at the threshold $T$ = 33 remains 0.5, the value we use for dimer discrimination throughout the paper. As mentioned, the same threshold value also yields the maximum Matthew correlation coefficient (**Table S3**).

### Impact of Small Interface on Prediction Success Rate

It is well known that the interface area is a very important factor for the discrimination between crystallographic and biological dimers as crystallographic interfaces are generally smaller (<1000 Å$^2$) than biologically relevant ones. However, some of the biological interfaces are also small, which makes discrimination difficult. Since docking programs are in general less successful in predicting complexes with small interface areas, it was suggested by one of the reviewers that the successful identification of monomers might be a result of the inability of docking to identify correct small interfaces. In order to investigate this potential artifact, we have analyzed ClusPro, PISA, and EPPIC results for several interface-area ranges. The analysis was performed on the test set (783 proteins). Predictions were separately analyzed for interface areas below 600, 800, and 1000 Å$^2$ (**Table S15**). Results show that the identification of small interface area biological dimers is indeed difficult, and for <600 Å$^2$ interface the success rate with ClusPro is only 23.5% (4 out of the 17 cases). However, EPPIC and PISA have exactly the same success rate, thus the low success rate is not caused by the failure of docking. In addition, since the overall percentage of biological dimers with such small interface is low (17 out of 783, thus 2.17%) , the overall success rate is over 90%, in spite of the inability to correctly identify most of the dimers. For interface areas below 800 and 1000 Å$^2$ finding biological dimers is still difficult, and all three methods still produce relatively weak results, with less than 50% success rates in all but one cases. However, ClusPro actually yields better discrimination for biological dimers than the other two methods (**Table S15**), again confirming that the failures are not due to the difficulty of docking.

### Application to Transient Complexes

Transient protein–protein complexes dissociate and associate readily, often depending on the physiological condition or environment, and this behavior frequently plays an important role in biological processes. It is expected that determining the state of such complexes under normal conditions is fairly difficult. We applied the three methods studied in this paper to the sets of transient homomultimers collected by Nooren and Thornton [1] and by Dey et al. [2]. As shown in **Table S16**, the average interface area is 855.1 Å$^2$, and only 3 of the 24 complexes by Nooren and Thornton [1] have interface area exceeding 1000 Å$^2$. Based on Cluspro, the average probability of being a dimer is 0.68, thus slightly shifted toward the dimer state. In **Table S17** we investigate the relationship between the biological active form as provided by Nooren and Thornton , and the assignment of multimeric state by ClusPro, EPPIC, and PISA. The function of the first 3 proteins in the Table (Lambda phage cro, corynebacterium diphtheria tox repressor, and mouse nuclear factor κB (NFκB P50 and P65, each with several structures) is DNA binding, and these proteins are active as dimers. In good agreement with this function, ClusPro predicts predominantly dimeric form for all but one (1nfk)

structures. According to EPPIC, the same structure and one more (5cro) are monomers. PISA predicts two NFκB structures as monomers, and does not reach conclusion in two more cases. In spite of these differences, all three programs reveal that most of the structures are homodimers. The next six proteins in Table S17 (interleukin-8, stromal cell-derived factor 1α, monocyte chemoattractant protein 1, stem cell factor cytokine, ciliary neurotrophic factor, and insulin) participate in extracellular, signaling, most likely acting in both monomeric and dimeric forms. Accordingly, ClusPro predict dimerization probabilities between 0.12 and 0.7. The biological active forms are somewhat uncertain for the remaining proteins in Table S17, and ClusPro predictions also vary, but in many cases are close to 0.5, reflecting the uncertainty of dimerization state assignment. As shown in **Table S18**, the three methods predict very similar percentages being in dimeric form.

To study the properties of transient homodimers, Dey et al. [2] built a list of 315 PDB entries containing the atomic coordinates of proteins shown by experiment to be homodimers in solution and in the crystal. Then, they identified cases where the literature indicates that the dimer is in equilibrium with the monomer; the 42 proteins shown in **Table S19** constitute a set of dimers marked “weak” to indicate that they dissociate easily. As for the set by Nooren and Thornton [1], the average interface area is small (817.2 $Å^2$), and only 7 of the 42 complexes have interface area exceeding 1000 $Å^2$. The average probability of being a biological dimer is 0.54, indicating almost the same frequency of dimeric and monomeric states. In contrast, the remaining 273 “others” type homodimers, listed in Table S20, have average surface area of 1922.8 $Å^2$, thus more than twice as large. The average probability of being a biological dimer is 0.75. As shown in **Tables S23** and **S24,** in the weak set all three methods predicts around 50 of biological dimers, whereas in the “others” set the fraction is about 85%. In both cases ClusPro predicts slightly more dimers than the other two methods.

**Table S1.** Training set PDB entries

| A. Biological homodimers[a] | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 12as | 1a3c | 1a4i | 1a4u | 1aa7 | 1ad3 | 1ade | 1af5 | 1afw | 1ajs |
| 1vlb | 1amk | 1aor | 1aq6 | 1auo | 1b3a | 1b5e | 1b67 | 1b8a | 1b8j |
| 1bam | 1bbh | 1bd0 | 1bif | 1biq | 1bis | 1bjw | 1bkp | 1bmd | 1brw |
| 1bsl | 1bsr | 1buo | 1bxg | 1bxk | 1cdc | 1cg2 | 1chm | 1cmb | 1cnz |
| 1coz | 1csh | 1ctt | 1cvu | 1czj | 1daa | 1dor | 1dpg | 1dqs | 1dxg |
| 1e98 | 1ebh | 1f13 | 1fip | 1fro | 1gvp | 1hhp | 1hjr | 1hss | 1hxp |
| 1icw | 1imb | 1isa | 1ivy | 1jhg | 1jsg | 1kba | 1kpf | 1lyn | 1m6p |
| 1mkb | 1mor | 1nox | 1nse | 1nsy | 1oac | 1opy | 1pgt | 1pre | 1qfh |
| 1qhi | 1qr2 | 1r2f | 1reg | 1rfb | 1rpo | 1ses | 1slt | 1smn | 1smt |
| 1sox | 1tc1 | 1tox | 1trk | 1uby | 1utg | 1vfr | 1vok | 1wtl | 1xso |
| 2arc | 2ccy | 2hdh | 2ilk | 2lig | 2mcg | 2nac | 2ohx | 2spc | 2sqc |
| 2tct | 2tgi | 3dap | 3sdh | 3ssi | 4kbp | 5csm | 5rub | 8prk | 9wga |
| B. Monomers (crystallographic dimers)[b] | | | | | | | | | |
| 13pk | 1a7v | 1ad5 | 1afk | 1ag9 | 1ah7 | 1ako | 1amu | 1atl | 1aw7 |
| 1ayl | 1b1j | 1b3j | 1bc2 | 1bea | 1bin | 1bkz | 1bs2 | 1byo | 1c02 |
| 1caq | 1ck7 | 1cki | 1clu | 1cqx | 1dsu | 1dys | 1e0s | 1ehy | 1epa |
| 1ewf | 1feh | 1fgk | 1fjm | 1fkd | 1fmt | 1g2a | 1gar | 1gjm | 1hf8 |
| 2j5x | 1ilr | 1kpt | 1kwa | 1mpg | 1mss | 1naw | 1np4 | 1pbg | 1pda |
| 1ppo | 1qaz | 1qci | 1qdm | 1qha | 1qjp | 1qme | 1qpa | 1qtq | 1rb3 |
| 1rhs | 1rne | 1shk | 1the | 1tht | 1toa | 1ton | 1urp | 1vbt | 1xgs |
| 256b | 256l | 2acy | 2atj | 2bc2 | 2bls | 2erc | 2g3p | 2ihl | 2mbr |
| 2scp | 2shp | 2tps | 2ugi | 3mht | 3pmg | 5tss | 830c | 8pti | |

[a] Biological homodimers from Baskaran et al. [3]
[b] Monomers (crystallographic dimers) from Baskaran et al. [4]

**Table S2.** Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the training set[a,b]

| Biological dimers | | | | Monomers (Crystallographic dimers) | | | |
|---|---|---|---|---|---|---|---|
| PDB ID | Interface area (Å²) | Nnn | Probability (dimer) | PDB ID | Interface area (Å²) | Nnn | Probability (dimer) |
| 12as | 1878.1 | 156 | 0.84 | 13pk | 1367.4 | 81 | 0.77 |
| 1a3c | 989.1 | 173 | 0.85 | 1a7v | 547.8 | 13 | 0.29 |
| 1a4i | 1354.6 | 114 | 0.82 | 1ad5 | 1053.1 | 9 | 0.24 |
| 1a4u | 2525.1 | 195 | 0.89 | 1afk | 818.5 | 4 | 0.18 |
| 1aa7 | 1093.8 | 46 | 0.60 | 1ag9 | 390.2 | 0 | 0.12 |
| 1ad3 | 3940.1 | 39 | 0.55 | 1ah7 | 949.4 | 21 | 0.39 |
| 1ade | 2699.0 | 107 | 0.81 | 1ako | 843.3 | 0 | 0.12 |
| 1af5 | 851.3 | 0 | 0.12 | 1amu | 679.6 | 0 | 0.12 |
| 1afw | 2388.7 | 123 | 0.82 | 1atl | 621.2 | 0 | 0.12 |
| 1ajs | 3436.9 | 74 | 0.74 | 1aw7 | 1145.9 | 5 | 0.19 |
| 1vlb | 1187.2 | 145 | 0.83 | 1ayl | 910.2 | 16 | 0.33 |
| 1amk | 1467.8 | 205 | 0.93 | 1b1j | 722.8 | 178 | 0.86 |
| 1aor | 1209.9 | 19 | 0.36 | 1b3j | 1630.4 | 102 | 0.81 |
| 1aq6 | 2220.5 | 176 | 0.86 | 1bc2 | 640.6 | 0 | 0.12 |
| 1auo | 663.7 | 0 | 0.12 | 1bea | 530.1 | 0 | 0.12 |
| 1b3a | 733.0 | 200 | 0.91 | 1bin | 553.7 | 0 | 0.12 |
| 1b5e | 2527.4 | 117 | 0.82 | 1bkz | 742.8 | 144 | 0.83 |
| 1b67 | 1595.9 | 283 | 1.00 | 1bs2 | 1113.6 | 31 | 0.49 |
| 1b8a | 4375.3 | 103 | 0.81 | 1byo | 483.6 | 0 | 0.12 |
| 1b8j | 3790.5 | 94 | 0.79 | 1c02 | 866.0 | 66 | 0.71 |
| 1bam | 750.0 | 128 | 0.83 | 1caq | 643.3 | 0 | 0.12 |
| 1bbh | 765.0 | 271 | 1.00 | 1ck7 | 1320.9 | 0 | 0.12 |
| 1bd0 | 3042.4 | 98 | 0.80 | 1cki | 1690.6 | 133 | 0.83 |
| 1bif | 889.7 | 6 | 0.20 | 1clu | 749.1 | 0 | 0.12 |
| 1biq | 3012.6 | 99 | 0.80 | 1cqx | 1109.5 | 0 | 0.12 |
| 1bis | 1478.5 | 205 | 0.93 | 1dsu | 635.4 | 1 | 0.13 |
| 1bjw | 2945.7 | 70 | 0.73 | 1dys | 765.3 | 25 | 0.43 |
| 1bkp | 2206.0 | 142 | 0.83 | 1e0s | 859.7 | 0 | 0.12 |
| 1bmd | 1590.4 | 253 | 1.00 | 1ehy | 696.4 | 92 | 0.79 |
| 1brw | 1060.5 | 249 | 1.00 | 1epa | 769.4 | 0 | 0.12 |
| 1bsl | 1893.9 | 158 | 0.84 | 1ewf | 947.4 | 0 | 0.12 |
| 1bsr | 1895.4 | 277 | 1.00 | 1feh | 1561.1 | 10 | 0.26 |
| 1buo | 1927.6 | 165 | 0.84 | 1fgk | 828.5 | 2 | 0.15 |
| 1bxg | 1039.6 | 71 | 0.73 | 1fjm | 641.7 | 0 | 0.12 |
| 1bxk | 1276.6 | 111 | 0.82 | 1fkd | 629.5 | 0 | 0.12 |
| 1cdc | 3837.9 | 70 | 0.73 | 1fmt | 962.3 | 30 | 0.48 |
| 1cg2 | 1298.3 | 73 | 0.74 | 1g2a | 573.6 | 0 | 0.12 |
| 1chm | 3230.1 | 70 | 0.73 | 1gar | 784.8 | 0 | 0.12 |
| 1cmb | 1796.3 | 481 | 1.00 | 1gjm | 895.8 | 0 | 0.12 |
| 1cnz | 2444.9 | 107 | 0.81 | 1hf8 | 1002.5 | 127 | 0.83 |
| 1coz | 1053.1 | 192 | 0.89 | 2j5x | 560.3 | 0 | 0.12 |
| 1csh | 4995.4 | 61 | 0.69 | 1ilr | 572.2 | 0 | 0.12 |
| 1ctt | 1933.3 | 134 | 0.83 | 1kpt | 432.9 | 9 | 0.24 |
| 1cvu | 2444.7 | 26 | 0.44 | 1kwa | 599.4 | 0 | 0.12 |
| 1czj | 741.3 | 7 | 0.22 | 1mpg | 987.2 | 31 | 0.49 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1daa | 2301.1 | 181 | 0.86 | 1mss | 1045.4 | 73 | 0.74 |
| 1dor | 2196.2 | 130 | 0.83 | 1naw | 1192.5 | 16 | 0.33 |
| 1dpg | 2278.7 | 167 | 0.84 | 1np4 | 731.3 | 1 | 0.13 |
| 1dqs | 1604.6 | 87 | 0.78 | 1pbg | 771.0 | 1 | 0.13 |
| 1dxg | 709.8 | 340 | 1.00 | 1pda | 881.2 | 4 | 0.18 |
| 1e98 | 770.4 | 230 | 1.00 | 1ppo | 847.2 | 0 | 0.12 |
| 1ebh | 1781.7 | 115 | 0.82 | 1qaz | 797.8 | 0 | 0.12 |
| 1f13 | 2563.6 | 57 | 0.67 | 1qci | 483.6 | 0 | 0.12 |
| 1fip | 1578.0 | 209 | 0.94 | 1qdm | 767.8 | 0 | 0.12 |
| 1fro | 3575.0 | 96 | 0.80 | 1qha | 1727.2 | 7 | 0.22 |
| 1gvp | 905.1 | 192 | 0.89 | 1qjp | 832.1 | 3 | 0.16 |
| 1hhp | 1596.7 | 281 | 1.00 | 1qme | 1271.9 | 15 | 0.32 |
| 1hjr | 962.0 | 83 | 0.77 | 1qpa | 822.9 | 32 | 0.49 |
| 1hss | 1095.5 | 64 | 0.70 | 1qtq | 715.7 | 11 | 0.27 |
| 1hxp | 3398.7 | 113 | 0.82 | 1rb3 | 614.9 | 0 | 0.12 |
| 1icw | 989.9 | 137 | 0.83 | 1rhs | 595.0 | 0 | 0.12 |
| 1imb | 1648.7 | 185 | 0.87 | 1rne | 1077.3 | 101 | 0.81 |
| 1isa | 919.0 | 180 | 0.86 | 1shk | 893.9 | 1 | 0.13 |
| 1ivy | 1586.2 | 141 | 0.83 | 1the | 1122.0 | 11 | 0.27 |
| 1jhg | 2225.9 | 349 | 1.00 | 1tht | 1049.3 | 134 | 0.83 |
| 1jsg | 789.3 | 146 | 0.83 | 1toa | 1294.4 | 27 | 0.45 |
| 1kba | 599.5 | 0 | 0.12 | 1ton | 712.8 | 21 | 0.39 |
| 1kpf | 1855.0 | 198 | 0.90 | 1urp | 906.7 | 0 | 0.12 |
| 1lyn | 942.1 | 39 | 0.55 | 1vbt | 642.8 | 3 | 0.16 |
| 1m6p | 1017.7 | 99 | 0.80 | 1xgs | 1177.2 | 74 | 0.74 |
| 1mkb | 1598.0 | 124 | 0.82 | 256b | 520.5 | 0 | 0.12 |
| 1mor | 2528.4 | 97 | 0.80 | 256l | 763.1 | 9 | 0.24 |
| 1nox | 2966.1 | 122 | 0.82 | 2acy | 541.4 | 58 | 0.68 |
| 1nse | 2674.6 | 102 | 0.81 | 2atj | 576.0 | 0 | 0.12 |
| 1nsy | 2583.3 | 120 | 0.82 | 2bc2 | 648.1 | 0 | 0.12 |
| 1oac | 7135.2 | 16 | 0.33 | 2bls | 706.0 | 8 | 0.23 |
| 1opy | 1044.8 | 65 | 0.71 | 2erc | 1364.0 | 1 | 0.13 |
| 1pgt | 1228.4 | 157 | 0.84 | 2g3p | 1407.3 | 31 | 0.49 |
| 1pre | 2280.7 | 33 | 0.50 | 2ihl | 708.5 | 47 | 0.61 |
| 1qfh | 2275.0 | 55 | 0.66 | 2mbr | 750.5 | 0 | 0.12 |
| 1qhi | 1698.8 | 103 | 0.81 | 2scp | 1115.1 | 81 | 0.77 |
| 1qr2 | 1917.0 | 130 | 0.83 | 2shp | 591.3 | 0 | 0.12 |
| 1r2f | 1741.9 | 127 | 0.83 | 2tps | 805.7 | 60 | 0.69 |
| 1reg | 676.5 | 0 | 0.12 | 2ugi | 738.4 | 2 | 0.15 |
| 1rfb | 2636.9 | 77 | 0.75 | 3mht | 667.9 | 173 | 0.85 |
| 1rpo | 1398.9 | 182 | 0.86 | 3pmg | 899.1 | 13 | 0.29 |
| 1ses | 2229.6 | 107 | 0.81 | 5tss | 1369.6 | 31 | 0.49 |
| 1slt | 547.2 | 134 | 0.83 | 830c | 1207.8 | 69 | 0.73 |
| 1smn | 868.4 | 164 | 0.84 | 8pti | 688.5 | 7 | 0.22 |
| 1smt | 1969.4 | 278 | 1.00 | | | | |
| 1sox | 1410.1 | 87 | 0.78 | | | | |
| 1tc1 | 1505.7 | 92 | 0.79 | | | | |
| 1tox | 3703.5 | 86 | 0.78 | | | | |
| 1trk | 4418.3 | 54 | 0.65 | | | | |
| 1uby | 2162.4 | 135 | 0.83 | | | | |
| 1utg | 1464.2 | 177 | 0.86 | | | | |
| 1vfr | 3355.7 | 73 | 0.74 | | | | |
| 1vok | 1582.6 | 159 | 0.84 | | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 1wtl | 686.4 | 96 | 0.80 | | | | |
| 1xso | 666.8 | 102 | 0.81 | | | | |
| 2arc | 810.3 | 83 | 0.77 | | | | |
| 2ccy | 807.3 | 175 | 0.85 | | | | |
| 2hdh | 1604.4 | 260 | 1.00 | | | | |
| 2ilk | 4479.7 | 43 | 0.58 | | | | |
| 2lig | 1581.1 | 47 | 0.61 | | | | |
| 2mcg | 1631.8 | 80 | 0.76 | | | | |
| 2nac | 3793.4 | 180 | 0.86 | | | | |
| 2ohx | 1685.1 | 339 | 1.00 | | | | |
| 2spc | 2513.5 | 57 | 0.67 | | | | |
| 2sqc | 805.8 | 0 | 0.12 | | | | |
| 2tct | 2612.3 | 137 | 0.83 | | | | |
| 2tgi | 1260.4 | 145 | 0.83 | | | | |
| 3dap | 2653.4 | 154 | 0.84 | | | | |
| 3sdh | 879.3 | 104 | 0.81 | | | | |
| 3ssi | 838.4 | 115 | 0.82 | | | | |
| 4kbp | 1467.9 | 125 | 0.83 | | | | |
| 5csm | 2000.1 | 38 | 0.54 | | | | |
| 5rub | 2829.1 | 99 | 0.80 | | | | |
| 8prk | 968.0 | 239 | 1.00 | | | | |
| 9wga | 2298.4 | 151 | 0.83 | | | | |
| Average | 1923.7 | 129.5 | 0.77 | Average | 863.7 | 25.3 | 0.32 |
| Std Dev | 1097.2 | 82.2 | 0.20 | Std Dev | 294.6 | 42.4 | 0.26 |

[a] Biological homodimers from Baskaran et al. [3]
[b] Monomers (crystallographic dimers) fro Baskaran et al. [4]

**Table S3.** MCC value as function of the threshold T[a]

| Threshold T | MCC |
|---|---|
| 20 | 0.64 |
| 21 | 0.64 |
| 22 | 0.66 |
| 23 | 0.66 |
| 24 | 0.66 |
| 25 | 0.66 |
| 26 | 0.67 |
| 27 | 0.66 |
| 28 | 0.67 |
| 29 | 0.67 |
| 30 | 0.67 |
| 31 | 0.68 |
| 32 | 0.72 |
| 33 | 0.73 |
| 34 | 0.72 |
| 35 | 0.72 |
| 36 | 0.72 |
| 37 | 0.72 |
| 38 | 0.72 |
| 39 | 0.71 |
| 40 | 0.69 |
| 41 | 0.69 |
| 42 | 0.69 |
| 43 | 0.69 |
| 44 | 0.68 |
| 45 | 0.68 |
| 46 | 0.68 |
| 47 | 0.67 |
| 48 | 0.67 |
| 49 | 0.67 |
| 50 | 0.67 |
| 51 | 0.67 |
| 52 | 0.67 |
| 53 | 0.67 |
| 54 | 0.67 |
| 55 | 0.66 |
| 56 | 0.65 |
| 57 | 0.65 |
| 58 | 0.63 |
| 59 | 0.64 |
| 60 | 0.64 |

[a] MCC: Matthews correlation coefficient

**Table S4.** Classification of training set dimers by three methods[a, b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 12as | 0.84 | bio | dimer | stable |
| 1a3c | 0.85 | bio | dimer | stable |
| 1a4i | 0.82 | bio | dimer | stable |
| 1a4u | 0.89 | bio | dimer | stable |
| 1aa7 | 0.6 | bio | monomer | stable |
| 1ad3 | 0.55 | bio | dimer | stable |
| 1ade | 0.81 | bio | dimer | stable |
| 1af5 | 0.12 | bio | dimer | stable |
| 1afw | 0.82 | bio | dimer | stable |
| 1ajs | 0.74 | bio | dimer | stable |
| 1vlb | 0.83 | bio | monomer | stable |
| 1amk | 0.93 | bio | dimer | stable |
| 1aor | 0.36 | bio | dimer | stable |
| 1aq6 | 0.86 | bio | dimer | stable |
| 1auo | 0.12 | bio | dimer | stable |
| 1b3a | 0.91 | bio | dimer | stable |
| 1b5e | 0.82 | bio | dimer | stable |
| 1b67 | 1 | xtal | dimer | stable |
| 1b8a | 0.81 | bio | dimer | stable |
| 1b8j | 0.79 | bio | dimer | stable |
| 1bam | 0.83 | xtal | dimer | uncertain |
| 1bbh | 1 | bio | dimer | stable |
| 1bd0 | 0.8 | bio | dimer | stable |
| 1bif | 0.2 | xtal | monomer | stable |
| 1biq | 0.8 | bio | dimer | stable |
| 1bis | 0.93 | bio | dimer | stable |
| 1bjw | 0.73 | bio | dimer | stable |
| 1bkp | 0.83 | bio | dimer | stable |
| 1bmd | 1 | bio | dimer | stable |
| 1brw | 1 | bio | dimer | stable |
| 1bsl | 0.84 | bio | dimer | stable |
| 1bsr | 1 | bio | tetramer | stable |
| 1buo | 0.84 | bio | dimer | stable |
| 1bxg | 0.73 | bio | dimer | uncertain |
| 1bxk | 0.82 | bio | dimer | stable |
| 1cdc | 0.73 | bio | dimer | stable |
| 1cg2 | 0.74 | bio | tetramer | stable |
| 1chm | 0.73 | bio | dimer | stable |
| 1cmb | 1 | bio | dimer | stable |
| 1cnz | 0.81 | bio | dimer | stable |
| 1coz | 0.89 | bio | dimer | stable |
| 1csh | 0.69 | bio | dimer | stable |
| 1ctt | 0.83 | bio | dimer | stable |
| 1cvu | 0.44 | bio | trimer | stable |
| 1czj | 0.22 | bio | dimer | stable |
| 1daa | 0.86 | bio | dimer | stable |
| 1dor | 0.83 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1dpg | 0.84 | bio | dimer | stable |
| 1dqs | 0.78 | bio | dimer | stable |
| 1dxg | 1 | bio | dimer | stable |
| 1e98 | 1 | bio | dimer | stable |
| 1ebh | 0.82 | bio | dimer | stable |
| 1f13 | 0.67 | bio | dimer | stable |
| 1fip | 0.94 | bio | tetramer | stable |
| 1fro | 0.8 | bio | dimer | stable |
| 1gvp | 0.89 | bio | dimer | stable |
| 1hhp | 1 | bio | dimer | stable |
| 1hjr | 0.77 | bio | dimer | stable |
| 1hss | 0.7 | bio | dimer | stable |
| 1hxp | 0.82 | bio | dimer | stable |
| 1icw | 0.83 | bio | dimer | stable |
| 1imb | 0.87 | xtal | dimer | stable |
| 1isa | 0.86 | bio | dimer | stable |
| 1ivy | 0.83 | bio | dimer | stable |
| 1jhg | 1 | bio | dimer | stable |
| 1jsg | 0.83 | bio | tetramer | stable |
| 1kba | 0.12 | bio | dimer | stable |
| 1kpf | 0.9 | bio | dimer | stable |
| 1lyn | 0.55 | bio | dimer | stable |
| 1m6p | 0.8 | bio | dimer | stable |
| 1mkb | 0.82 | bio | dimer | stable |
| 1mor | 0.8 | bio | dimer | stable |
| 1nox | 0.82 | bio | dimer | stable |
| 1nse | 0.81 | bio | dimer | stable |
| 1nsy | 0.82 | bio | dimer | stable |
| 1oac | 0.33 | bio | dimer | stable |
| 1opy | 0.71 | xtal | dimer | stable |
| 1pgt | 0.84 | bio | dimer | stable |
| 1pre | 0.5 | bio | dimer | stable |
| 1qfh | 0.66 | bio | dimer | stable |
| 1qhi | 0.81 | bio | dimer | stable |
| 1qr2 | 0.83 | bio | dimer | stable |
| 1r2f | 0.83 | bio | dimer | stable |
| 1reg | 0.12 | bio | dimer | stable |
| 1rfb | 0.75 | bio | dimer | stable |
| 1rpo | 0.86 | bio | dimer | stable |
| 1ses | 0.81 | bio | dimer | stable |
| 1slt | 0.83 | xtal | monomer | stable |
| 1smn | 0.84 | xtal | dimer | uncertain |
| 1smt | 1 | bio | dimer | stable |
| 1sox | 0.78 | bio | dimer | stable |
| 1tc1 | 0.79 | bio | dimer | stable |
| 1tox | 0.78 | bio | dimer | stable |
| 1trk | 0.65 | bio | dimer | stable |
| 1uby | 0.83 | bio | dimer | stable |
| 1utg | 0.86 | bio | dimer | stable |
| 1vfr | 0.74 | bio | dimer | stable |
| 1vok | 0.84 | bio | tetramer | stable |
| 1wtl | 0.8 | bio | dimer | stable |
| 1xso | 0.81 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 2arc | 0.77 | bio | monomer | stable |
| 2ccy | 0.85 | bio | dimer | stable |
| 2hdh | 1 | bio | dimer | stable |
| 2ilk | 0.58 | bio | dimer | stable |
| 2lig | 0.61 | bio | dimer | stable |
| 2mcg | 0.76 | bio | dimer | stable |
| 2nac | 0.86 | bio | dimer | stable |
| 2ohx | 1 | xtal | dimer | stable |
| 2spc | 0.67 | bio | dimer | stable |
| 2sqc | 0.12 | xtal | monomer | stable |
| 2tct | 0.83 | bio | dimer | stable |
| 2tgi | 0.83 | bio | dimer | stable |
| 3dap | 0.84 | bio | dimer | stable |
| 3sdh | 0.81 | bio | dimer | stable |
| 3ssi | 0.82 | bio | dimer | stable |
| 4kbp | 0.83 | bio | tetramer | stable |
| 5csm | 0.54 | bio | dimer | stable |
| 5rub | 0.8 | bio | dimer | stable |
| 8prk | 1 | bio | dimer | stable |
| 9wga | 0.83 | bio | dimer | stable |

[a] yellow: incorrect classification
[b] biological homodimers from Baskaran et al. [3]

**Table S5.** Classification of training set monomers by three methods[a,b]

| PDB ID | ClusPro Probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 13pk | 0.77 | xtal | dimer | stable |
| 1a7v | 0.29 | xtal | monomer | stable |
| 1ad5 | 0.24 | xtal | dimer | uncertain |
| 1afk | 0.18 | xtal | dimer | uncertain |
| 1ag9 | 0.12 | xtal | dimer | stable |
| 1ah7 | 0.39 | bio | monomer | stable |
| 1ako | 0.12 | xtal | dimer | stable |
| 1amu | 0.12 | xtal | monomer | stable |
| 1atl | 0.12 | xtal | monomer | stable |
| 1aw7 | 0.19 | xtal | monomer | stable |
| 1ayl | 0.33 | xtal | monomer | stable |
| 1b1j | 0.86 | xtal | monomer | stable |
| 1b3j | 0.81 | xtal | dimer | uncertain |
| 1bc2 | 0.12 | bio | monomer | stable |
| 1bea | 0.12 | xtal | tetramer | uncertain |
| 1bin | 0.12 | xtal | dimer | uncertain |
| 1bkz | 0.83 | bio | monomer | stable |
| 1bs2 | 0.49 | xtal | dimer | uncertain |
| 1byo | 0.12 | xtal | monomer | stable |
| 1c02 | 0.71 | bio | dimer | stable |
| 1caq | 0.12 | bio | dimer | stable |
| 1ck7 | 0.12 | xtal | dimer | stable |
| 1cki | 0.83 | xtal | dimer | stable |
| 1clu | 0.12 | xtal | monomer | stable |
| 1cqx | 0.12 | bio | dimer | stable |
| 1dsu | 0.13 | xtal | monomer | stable |
| 1dys | 0.43 | xtal | monomer | stable |
| 1e0s | 0.12 | xtal | dimer | stable |
| 1ehy | 0.79 | bio | tetramer | stable |
| 1epa | 0.12 | xtal | dimer | stable |
| 1ewf | 0.12 | xtal | monomer | stable |
| 1feh | 0.26 | xtal | dimer | uncertain |
| 1fgk | 0.15 | xtal | monomer | stable |
| 1fjm | 0.12 | bio | monomer | stable |
| 1fkd | 0.12 | xtal | tetramer | stable |
| 1fmt | 0.48 | xtal | monomer | stable |
| 1g2a | 0.12 | xtal | monomer | stable |
| 1gar | 0.12 | xtal | dimer | stable |
| 1gjm | 0.12 | xtal | monomer | stable |
| 1hf8 | 0.83 | xtal | dimer | stable |
| 2j5x | 0.12 | xtal | monomer | stable |
| 1ilr | 0.12 | xtal | monomer | stable |
| 1kpt | 0.24 | xtal | monomer | stable |
| 1kwa | 0.12 | bio | tetramer | stable |
| 1mpg | 0.49 | xtal | dimer | stable |
| 1mss | 0.74 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1naw | 0.33 | bio | tetramer | stable |
| 1np4 | 0.13 | xtal | dimer | uncertain |
| 1pbg | 0.13 | xtal | dimer | uncertain |
| 1pda | 0.18 | xtal | monomer | stable |
| 1ppo | 0.12 | xtal | dimer | stable |
| 1qaz | 0.12 | xtal | monomer | stable |
| 1qci | 0.12 | xtal | monomer | stable |
| 1qdm | 0.12 | xtal | trimer | uncertain |
| 1qha | 0.22 | bio | monomer | stable |
| 1qjp | 0.16 | bio | monomer | stable |
| 1qme | 0.32 | xtal | monomer | stable |
| 1qpa | 0.49 | xtal | dimer | stable |
| 1qtq | 0.27 | xtal | dimer | stable |
| 1rb3 | 0.12 | xtal | monomer | stable |
| 1rhs | 0.12 | xtal | monomer | stable |
| 1rne | 0.81 | xtal | dimer | stable |
| 1shk | 0.13 | xtal | dimer | stable |
| 1the | 0.27 | xtal | dimer | stable |
| 1tht | 0.83 | xtal | dimer | stable |
| 1toa | 0.45 | bio | dimer | stable |
| 1ton | 0.39 | xtal | dimer | stable |
| 1urp | 0.12 | xtal | monomer | stable |
| 1vbt | 0.16 | bio | monomer | stable |
| 1xgs | 0.74 | xtal | monomer | stable |
| 256b | 0.12 | xtal | monomer | stable |
| 256l | 0.24 | xtal | monomer | stable |
| 2acy | 0.68 | bio | monomer | stable |
| 2atj | 0.12 | xtal | monomer | stable |
| 2bc2 | 0.12 | bio | dimer | stable |
| 2bls | 0.23 | xtal | dimer | uncertain |
| 2erc | 0.13 | xtal | dimer | stable |
| 2g3p | 0.49 | xtal | dimer | stable |
| 2ihl | 0.61 | xtal | monomer | stable |
| 2mbr | 0.12 | bio | monomer | stable |
| 2scp | 0.77 | bio | dimer | uncertain |
| 2shp | 0.12 | xtal | monomer | stable |
| 2tps | 0.69 | xtal | monomer | stable |
| 2ugi | 0.15 | xtal | dimer | stable |
| 3mht | 0.85 | xtal | trimer | stable |
| 3pmg | 0.29 | xtal | monomer | stable |
| 5tss | 0.49 | xtal | dimer | uncertain |
| 830c | 0.73 | bio | tetramer | stable |
| 8pti | 0.22 | bio | dimer | stable |

[a] yellow: incorrect classification
[b] monomers (crystallographic dimers) from Baskaran et al. [4]

**Table S5.** MCC value as function of the threshold T[a]

| Threshold T | MCC |
|---|---|
| 20 | 0.64 |
| 21 | 0.64 |
| 22 | 0.66 |
| 23 | 0.66 |
| 24 | 0.66 |
| 25 | 0.66 |
| 26 | 0.67 |
| 27 | 0.66 |
| 28 | 0.67 |
| 29 | 0.67 |
| 30 | 0.67 |
| 31 | 0.68 |
| 32 | 0.72 |
| 33 | 0.73 |
| 34 | 0.72 |
| 35 | 0.72 |
| 36 | 0.72 |
| 37 | 0.72 |
| 38 | 0.72 |
| 39 | 0.71 |
| 40 | 0.69 |
| 41 | 0.69 |
| 42 | 0.69 |
| 43 | 0.69 |
| 44 | 0.68 |
| 45 | 0.68 |
| 46 | 0.68 |
| 47 | 0.67 |
| 48 | 0.67 |
| 49 | 0.67 |
| 50 | 0.67 |
| 51 | 0.67 |
| 52 | 0.67 |
| 53 | 0.67 |
| 54 | 0.67 |
| 55 | 0.66 |
| 56 | 0.65 |
| 57 | 0.65 |
| 58 | 0.63 |
| 59 | 0.64 |
| 60 | 0.64 |

[a] MCC: Matthews correlation coefficient

**Table S6.** Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the DC Bio and DC Xtal sets[a]

| Biological dimers | | | | Crystallographic dimers | | | |
|---|---|---|---|---|---|---|---|
| PDB ID | Interface area (Å²) | Nnn | Probability (dimer) | PDB ID | Interface area (Å²) | Nnn | Probability (dimer) |
| 2fwv | 2088.9 | 225 | 1.00 | 1ejd | 1215.9 | 16 | 0.33 |
| 1v2x | 1684.6 | 178 | 0.86 | 1gpi | 1043.3 | 51 | 0.64 |
| 1pkh | 1624.2 | 93 | 0.79 | 1j96 | 1217.0 | 37 | 0.54 |
| 1r5y | 1551.5 | 150 | 0.83 | 1lqt | 1099.9 | 0 | 0.12 |
| 1kq3 | 1487.5 | 129 | 0.83 | 1lxk | 1028.7 | 1 | 0.13 |
| 1jq5 | 1325.9 | 191 | 0.88 | 1n45 | 1089.3 | 11 | 0.27 |
| 2h7i | 1468.8 | 99 | 0.80 | 1pp3 | 1106.8 | 23 | 0.41 |
| 2nzl | 1299.0 | 177 | 0.86 | 1s83 | 925.1 | 1 | 0.13 |
| 1uj6 | 1257.5 | 137 | 0.83 | 1so7 | 1189.4 | 15 | 0.32 |
| 1ju3 | 1266.4 | 49 | 0.62 | 1ueb | 1150.0 | 26 | 0.44 |
| 1sml | 1253.3 | 37 | 0.54 | 1w9q | 1000.7 | 57 | 0.67 |
| 3fah | 1236.5 | 153 | 0.83 | 1wly | 1144.8 | 57 | 0.67 |
| 1lzl | 1207.4 | 219 | 0.99 | 1xgk | 1014.5 | 5 | 0.19 |
| 3iue | 1106.1 | 101 | 0.81 | 1ynq | 1100.6 | 5 | 0.19 |
| 1vk5 | 1110.5 | 69 | 0.73 | 2cki | 1203.5 | 79 | 0.76 |
| 2exb | 1895.8 | 41 | 0.57 | 2eyi | 1112.3 | 0 | 0.12 |
| 3a2q | 1745.5 | 156 | 0.84 | 2f37 | 1163.9 | 0 | 0.12 |
| 1s2z | 1619.4 | 170 | 0.85 | 2gas | 1561.6 | 89 | 0.79 |
| 2z1n | 1578.5 | 91 | 0.79 | 2hlq | 1071.7 | 21 | 0.39 |
| 2vef | 1544.2 | 204 | 0.92 | 2ipi | 1330.5 | 0 | 0.12 |
| 1bs1 | 1455.5 | 237 | 1.00 | 2j0p | 1016.7 | 189 | 0.88 |
| 3lw6 | 1013.0 | 200 | 0.91 | 2j46 | 1152.0 | 6 | 0.20 |
| 2vr4 | 1278.8 | 55 | 0.66 | 2ow9 | 1179.4 | 65 | 0.71 |
| 1x7v | 1190.5 | 220 | 1.00 | 2q7d | 1782.7 | 46 | 0.60 |
| 1f2d | 1890.4 | 63 | 0.70 | 2w20 | 1090.3 | 0 | 0.12 |
| 1lw4 | 1772.9 | 87 | 0.78 | 2wbf | 1204.3 | 2 | 0.15 |
| 1n8p | 1932.3 | 1 | 0.13 | 2wbq | 1521.9 | 86 | 0.78 |
| 1qop | 1536.3 | 85 | 0.78 | 2wsa | 1002.4 | 0 | 0.12 |
| 2aq6 | 1188.1 | 59 | 0.68 | 2xov | 1144.4 | 0 | 0.12 |
| 2bhs | 1484.0 | 96 | 0.80 | 2yz1 | 1372.0 | 199 | 0.91 |
| 2cft | 946.6 | 92 | 0.79 | 2z6o | 1156.5 | 18 | 0.35 |
| 2e7j | 1671.2 | 113 | 0.82 | 3aap | 1382.8 | 139 | 0.83 |
| 2ecq | 1626.5 | 68 | 0.72 | 3b37 | 1150.4 | 2 | 0.15 |
| 2rkb | 1104.5 | 134 | 0.83 | 3c8y | 1525.0 | 13 | 0.29 |
| 1eej | 856.9 | 177 | 0.86 | 3cj1 | 1122.9 | 37 | 0.54 |
| 1o17 | 932.1 | 143 | 0.83 | 3cu9 | 1085.4 | 2 | 0.15 |
| 3d36 | 1660.8 | 97 | 0.80 | 3fwk | 1044.4 | 0 | 0.12 |
| 3r0n | 884.7 | 82 | 0.77 | 3gkj | 992.4 | 32 | 0.49 |
| 3da8 | 867.3 | 11 | 0.27 | 3go5 | 1049.8 | 0 | 0.12 |
| 2c4w | 872.9 | 15 | 0.32 | 3gvo | 1208.0 | 65 | 0.71 |
| 3jrz | 932.7 | 232 | 1.00 | 3h30 | 1310.1 | 4 | 0.18 |
| 2wxd | 954.3 | 82 | 0.77 | 3hzl | 1000.0 | 38 | 0.54 |
| 2d0d | 1003.5 | 118 | 0.82 | 3kk8 | 1287.3 | 143 | 0.83 |
| 3cm3 | 1014.1 | 115 | 0.82 | 3m66 | 1006.6 | 2 | 0.15 |
| 3o1n | 1007.0 | 307 | 1.00 | 3mg1 | 1095.8 | 0 | 0.12 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 3h0n | 993.9 | 129 | 0.83 | 3mhz | 1530.8 | 0 | 0.12 |
| 2dvn | 1045.0 | 249 | 1.00 | 1lf2 | 2139.9 | 109 | 0.81 |
| 3ovp | 1067.4 | 129 | 0.83 | 2qb5 | 1797.0 | 49 | 0.62 |
| 2i7d | 1076.0 | 158 | 0.84 | 1zlq | 1653.2 | 13 | 0.29 |
| 2car | 1100.5 | 186 | 0.87 | 2yvw | 1516.4 | 65 | 0.71 |
| 3gus | 1215.6 | 167 | 0.84 | 1d3h | 1464.7 | 0 | 0.12 |
| 3jyo | 1224.2 | 279 | 1.00 | 2e1v | 1657.8 | 161 | 0.84 |
| 1uz3 | 1196.3 | 105 | 0.81 | 3n5c | 1455.7 | 147 | 0.83 |
| 2wtm | 1241.9 | 125 | 0.83 | 2wbm | 1441.3 | 62 | 0.70 |
| 2a5l | 1217.2 | 43 | 0.58 | 3c1d | 1429.8 | 49 | 0.62 |
| 2y39 | 1285.5 | 125 | 0.83 | 1ndb | 1383.0 | 0 | 0.12 |
| 2ab0 | 1290.6 | 97 | 0.80 | 2x26 | 1369.3 | 158 | 0.84 |
| 3epw | 1302.4 | 31 | 0.49 | 3kh7 | 1329.5 | 114 | 0.82 |
| 2vvt | 1328.8 | 16 | 0.33 | 1toa | 1294.4 | 27 | 0.45 |
| 1p5f | 1339.3 | 156 | 0.84 | 1ffr | 1223.4 | 76 | 0.75 |
| 3itf | 1392.3 | 80 | 0.76 | 1vqq | 1173.4 | 2 | 0.15 |
| 3kd2 | 1365.8 | 149 | 0.83 | 1n4g | 1161.5 | 101 | 0.81 |
| 2y27 | 1355.8 | 154 | 0.84 | 3ita | 1139.6 | 13 | 0.29 |
| | | | | 1woq | 1130.0 | 120 | 0.82 |
| | | | | 1cqx | 1109.5 | 0 | 0.12 |
| | | | | 2eqa | 1106.3 | 17 | 0.34 |
| | | | | 3mhj | 1098.5 | 8 | 0.23 |
| | | | | 2fgz | 1092.2 | 1 | 0.13 |
| | | | | 1fpo | 1080.0 | 0 | 0.12 |
| | | | | 3lvd | 996.1 | 46 | 0.60 |
| | | | | 3irb | 1075.3 | 64 | 0.70 |
| | | | | 1utj | 986.3 | 0 | 0.12 |
| | | | | 3f0o | 1040.1 | 9 | 0.24 |
| | | | | 2h44 | 1041.1 | 312 | 1.00 |
| | | | | 1t8g | 1026.1 | 0 | 0.12 |
| | | | | 1g6a | 1021.4 | 9 | 0.24 |
| | | | | 2zyr | 1010.6 | 32 | 0.49 |
| | | | | 3els | 949.9 | 15 | 0.32 |
| Average | 1309.0 | 126.0 | 0.78 | Average | 1212.5 | 43.1 | 0.42 |
| Std Dev | 293.8 | 68.0 | 0.18 | Std Dev | 225.4 | 58.8 | 0.28 |

[a] DC Bio and DC Xtal sets from Duarte et al. [5]

**Table S7**. Classification of DC Bio set by three methods[a, b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 2fwv | 1.00 | bio | tetramer | stable |
| 1v2x | 0.86 | bio | dimer | stable |
| 1pkh | 0.79 | bio | hexamer | stable |
| 1r5y | 0.83 | bio | dimer | stable |
| 1kq3 | 0.83 | bio | octomer | stable |
| 1jq5 | 0.88 | bio | octomer | stable |
| 2h7i | 0.80 | bio | tetramer | stable |
| 2nzl | 0.86 | bio | tetramer | stable |
| 1uj6 | 0.83 | bio | dimer | stable |
| 1ju3 | 0.62 | xtal | dimer | stable |
| 1sml | 0.54 | bio | tetramer | stable |
| 3fah | 0.83 | bio | dimer | stable |
| 1lzl | 0.99 | bio | dimer | stable |
| 3iue | 0.81 | bio | monomer | stable |
| 1vk5 | 0.73 | bio | dimer | stable |
| 2exb | 0.57 | bio | dimer | stable |
| 3a2q | 0.84 | bio | dimer | stable |
| 1s2z | 0.85 | bio | tetramer | stable |
| 2z1n | 0.79 | bio | tetramer | stable |
| 2vef | 0.92 | bio | dimer | stable |
| 1bs1 | 1.00 | bio | dimer | stable |
| 3lw6 | 0.91 | bio | monomer | stable |
| 2vr4 | 0.66 | bio | dimer | uncertain |
| 1x7v | 1.00 | bio | hexamer | stable |
| 1f2d | 0.70 | bio | dimer | stable |
| 1lw4 | 0.78 | bio | tetramer | stable |
| 1n8p | 0.13 | bio | tetramer | stable |
| 1qop | 0.78 | bio | tetramer | stable |
| 2aq6 | 0.68 | bio | dimer | stable |
| 2bhs | 0.80 | bio | dimer | stable |
| 2cft | 0.79 | bio | dimer | stable |
| 2e7j | 0.82 | bio | dimer | stable |
| 2ecq | 0.72 | xtal | dimer | stable |
| 2rkb | 0.83 | bio | dimer | stable |
| 1eej | 0.86 | bio | dimer | stable |
| 1o17 | 0.83 | xtal | dimer | stable |
| 3d36 | 0.80 | bio | hexamer | stable |
| 3r0n | 0.77 | bio | dimer | stable |
| 3da8 | 0.27 | bio | dimer | stable |
| 2c4w | 0.32 | bio | dodecamer | stable |
| 3jrz | 1.00 | bio | dimer | stable |
| 2wxd | 0.77 | bio | dimer | stable |
| 2d0d | 0.82 | bio | dimer | uncertain |
| 3cm3 | 0.82 | bio | dimer | stable |
| 3o1n | 1.00 | bio | dimer | stable |
| 3h0n | 0.83 | bio | dimer | stable |
| 2dvn | 1.00 | bio | tetramer | stable |

| | | | | |
|---|---|---|---|---|
| 3ovp | 0.83 | bio | dimer | stable |
| 2i7d | 0.84 | bio | dimer | stable |
| 2car | 0.87 | bio | dimer | stable |
| 3gus | 0.84 | bio | dimer | stable |
| 3jyo | 1.00 | bio | dimer | stable |
| 1uz3 | 0.81 | bio | dimer | stable |
| 2wtm | 0.83 | xtal | dimer | stable |
| 2a5l | 0.58 | bio | tetramer | stable |
| 2y39 | 0.83 | bio | dimer | stable |
| 2ab0 | 0.80 | bio | dimer | stable |
| 3epw | 0.49 | bio | dimer | stable |
| 2vvt | 0.33 | bio | dimer | stable |
| 1p5f | 0.84 | bio | dimer | stable |
| 3itf | 0.76 | bio | dimer | stable |
| 3kd2 | 0.83 | bio | dimer | stable |
| 2y27 | 0.84 | bio | dimer | stable |

[a] yellow: incorrect classification

[a] DC Bio and DC Xtal sets from Duarte et al. [5]

**Table S8.** Classification of DC Xtal set by three methods[a,b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 1ejd | 0.33 | bio | tetramer | stable |
| 1gpi | 0.64 | xtal | monomer | stable |
| 1j96 | 0.54 | xtal | monomer | stable |
| 1lqt | 0.12 | xtal | monomer | stable |
| 1lxk | 0.13 | xtal | monomer | stable |
| 1n45 | 0.27 | xtal | monomer | stable |
| 1pp3 | 0.41 | xtal | monomer | stable |
| 1s83 | 0.13 | xtal | monomer | stable |
| 1so7 | 0.32 | xtal | monomer | stable |
| 1ueb | 0.44 | xtal | dimer | stable |
| 1w9q | 0.67 | bio | trimer | stable |
| 1wly | 0.67 | bio | dimer | stable |
| 1xgk | 0.19 | bio | dimer | stable |
| 1ynq | 0.19 | xtal | dimer | stable |
| 2cki | 0.76 | xtal | dimer | stable |
| 2eyi | 0.12 | xtal | monomer | stable |
| 2f37 | 0.12 | xtal | monomer | stable |
| 2gas | 0.79 | xtal | dimer | stable |
| 2hlq | 0.39 | xtal | monomer | stable |
| 2ipi | 0.12 | bio | monomer | stable |
| 2j0p | 0.88 | bio | monomer | stable |
| 2j46 | 0.20 | xtal | monomer | stable |
| 2ow9 | 0.71 | bio | tetramer | stable |
| 2q7d | 0.60 | xtal | dimer | stable |
| 2w20 | 0.12 | xtal | monomer | stable |
| 2wbf | 0.15 | xtal | monomer | stable |
| 2wbq | 0.78 | bio | dimer | stable |
| 2wsa | 0.12 | xtal | monomer | stable |
| 2xov | 0.12 | bio | monomer | stable |
| 2yz1 | 0.91 | bio | dimer | stable |
| 2z6o | 0.35 | xtal | monomer | stable |
| 3aap | 0.83 | bio | monomer | stable |
| 3b37 | 0.15 | xtal | monomer | stable |
| 3c8y | 0.29 | xtal | monomer | stable |
| 3cj1 | 0.54 | xtal | monomer | stable |
| 3cu9 | 0.15 | xtal | dimer | stable |
| 3fwk | 0.12 | xtal | monomer | stable |
| 3gkj | 0.49 | bio | monomer | stable |
| 3go5 | 0.12 | xtal | monomer | stable |
| 3gvo | 0.71 | bio | monomer | stable |
| 3h30 | 0.18 | xtal | dimer | stable |
| 3hzl | 0.54 | bio | dimer | uncertain |
| 3kk8 | 0.83 | xtal | monomer | stable |
| 3m66 | 0.15 | xtal | monomer | stable |
| 3mg1 | 0.12 | xtal | monomer | stable |
| 3mhz | 0.12 | xtal | monomer | stable |
| 1lf2 | 0.81 | xtal | tetramer | stable |
| 2qb5 | 0.62 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 1zlq | 0.29 | xtal | dimer | stable |
| 2yvw | 0.71 | bio | dimer | stable |
| 1d3h | 0.12 | xtal | monomer | stable |
| 2e1v | 0.84 | xtal | dimer | stable |
| 3n5c | 0.83 | bio | dimer | stable |
| 2wbm | 0.70 | bio | tetramer | stable |
| 3c1d | 0.62 | xtal | dimer | stable |
| 1ndb | 0.12 | xtal | monomer | stable |
| 2x26 | 0.84 | xtal | monomer | stable |
| 3kh7 | 0.82 | bio | dimer | stable |
| 1toa | 0.45 | bio | dimer | stable |
| 1ffr | 0.75 | bio | monomer | stable |
| 1vqq | 0.15 | xtal | dimer | stable |
| 1n4g | 0.81 | bio | dimer | stable |
| 3ita | 0.29 | xtal | dimer | stable |
| 1woq | 0.82 | bio | dimer | stable |
| 1cqx | 0.12 | bio | dimer | stable |
| 2eqa | 0.34 | bio | monomer | stable |
| 3mhj | 0.23 | xtal | monomer | stable |
| 2fgz | 0.13 | xtal | monomer | stable |
| 1fpo | 0.12 | bio | trimer | stable |
| 3lvd | 0.60 | xtal | monomer | stable |
| 3irb | 0.70 | xtal | tetramer | stable |
| 1utj | 0.12 | xtal | monomer | stable |
| 3f0o | 0.24 | bio | dimer | stable |
| 2h44 | 1.00 | xtal | dimer | stable |
| 1t8g | 0.12 | xtal | octomer | stable |
| 1g6a | 0.24 | bio | dimer | stable |
| 2zyr | 0.49 | xtal | monomer | stable |
| 3els | 0.32 | xtal | hexamer | stable |

[a] yellow: incorrect classification

[a] DC Bio and DC Xtal sets from Duarte et al. [5]

**Table S9.** Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the test set[a]

| Biological dimers | | | | Crystallographic dimers | | | |
|---|---|---|---|---|---|---|---|
| PDB ID | Interface area (Å²) | Nnn | Probability (dimer) | PDB ID | Interface area (Å²) | Nnn | Probability (dimer) |
| 3w66 | 529.6 | 0 | 0.12 | 3w6r | 859.9 | 54 | 0.65 |
| 3w8g | 760.8 | 183 | 0.87 | 3w94 | 750.3 | 0 | 0.12 |
| 3we1 | 529.3 | 1 | 0.13 | 3w9g | 604.3 | 8 | 0.23 |
| 3wfi | 1028.6 | 316 | 1.00 | 3wbi | 1467.0 | 0 | 0.12 |
| 3wjk | 1722.6 | 192 | 0.89 | 3wbj | 1195.5 | 59 | 0.68 |
| 3wkw | 2891.9 | 81 | 0.77 | 3wdf | 546.3 | 42 | 0.58 |
| 3wmd | 1081.4 | 47 | 0.61 | 3wea | 445.6 | 0 | 0.12 |
| 3wo8 | 2446.6 | 104 | 0.81 | 3who | 567.0 | 1 | 0.13 |
| 3wpx | 992.8 | 181 | 0.86 | 3wj9 | 588.6 | 0 | 0.12 |
| 3wsc | 1566.2 | 1 | 0.13 | 3wo9 | 710.6 | 0 | 0.12 |
| 3wtz | 690.6 | 74 | 0.74 | 3wob | 460.8 | 1 | 0.13 |
| 3wu0 | 687.0 | 88 | 0.78 | 3wp3 | 644.0 | 0 | 0.12 |
| 3wva | 1517.9 | 140 | 0.83 | 3wp9 | 716.5 | 23 | 0.41 |
| 3wvb | 1521.0 | 155 | 0.84 | 3wpj | 566.9 | 0 | 0.12 |
| 3wvo | 1540.6 | 78 | 0.76 | 3wpy | 1100.1 | 5 | 0.19 |
| 3wvz | 2607.7 | 82 | 0.77 | 3wpz | 1118.5 | 25 | 0.43 |
| 3wx4 | 1220.4 | 159 | 0.84 | 3wrt | 490.3 | 0 | 0.12 |
| 3wxi | 1416.9 | 148 | 0.83 | 3wuq | 798.5 | 0 | 0.12 |
| 3wy7 | 2592.5 | 114 | 0.82 | 3wuy | 872.8 | 0 | 0.12 |
| 3wyb | 3216.7 | 96 | 0.80 | 3wv4 | 514.6 | 0 | 0.12 |
| 3wyd | 542.7 | 68 | 0.72 | 3wvf | 451.6 | 0 | 0.12 |
| 3wzg | 1066.5 | 164 | 0.84 | 3wvt | 589.1 | 0 | 0.12 |
| 4bhy | 1988.9 | 37 | 0.54 | 3wx5 | 403.3 | 0 | 0.12 |
| 4c7v | 3998.0 | 78 | 0.76 | 3wzt | 718.4 | 13 | 0.29 |
| 4c88 | 1107.9 | 94 | 0.79 | 3x0w | 595.8 | 0 | 0.12 |
| 4cbv | 1777.7 | 54 | 0.65 | 3zfm | 333.2 | 0 | 0.12 |
| 4chk | 743.5 | 49 | 0.62 | 3zfy | 404.9 | 0 | 0.12 |
| 4cij | 1458.2 | 37 | 0.54 | 3zk0 | 589.7 | 7 | 0.22 |
| 4ckk | 1761.7 | 55 | 0.66 | 3zlh | 1825.2 | 97 | 0.80 |
| 4ckn | 1371.7 | 82 | 0.77 | 3zm0 | 334.0 | 0 | 0.12 |
| 4cmz | 3689.9 | 220 | 1.00 | 3zm1 | 314.0 | 0 | 0.12 |
| 4cop | 489.0 | 131 | 0.83 | 3zm2 | 324.7 | 0 | 0.12 |
| 4cti | 2596.6 | 62 | 0.70 | 3zm3 | 381.8 | 0 | 0.12 |
| 4cu5 | 706.1 | 481 | 1.00 | 3zny | 564.5 | 0 | 0.12 |
| 4cw9 | 635.1 | 0 | 0.12 | 3zq3 | 748.1 | 10 | 0.26 |
| 4cwc | 1505.3 | 52 | 0.64 | 4bg0 | 892.2 | 0 | 0.12 |
| 4cwe | 1378.3 | 30 | 0.48 | 4bob | 354.0 | 0 | 0.12 |
| 4cxj | 2001.5 | 137 | 0.83 | 4bod | 453.0 | 0 | 0.12 |
| 4d28 | 1404.9 | 34 | 0.51 | 4bp8 | 1075.0 | 51 | 0.64 |
| 4d5s | 758.2 | 142 | 0.83 | 4bpf | 580.6 | 2 | 0.15 |
| 4d6k | 2270.1 | 227 | 1.00 | 4bpy | 426.5 | 0 | 0.12 |
| 4fb8 | 2682.2 | 108 | 0.81 | 4bxm | 584.7 | 0 | 0.12 |
| 4ihe | 1746.5 | 118 | 0.82 | 4c41 | 620.9 | 0 | 0.12 |
| 4j0e | 1685.2 | 213 | 0.96 | 4c5f | 599.5 | 0 | 0.12 |
| 4j0f | 1644.4 | 216 | 0.97 | 4c6r | 710.5 | 11 | 0.27 |
| 4j7a | 1116.5 | 110 | 0.82 | 4cbe | 896.0 | 0 | 0.12 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4j7r | 1911.8 | 232 | 1.00 | 4cbh | 1171.6 | 0 | 0.12 |
| 4jgm | 698.2 | 0 | 0.12 | 4cbi | 1177.1 | 0 | 0.12 |
| 4jp2 | 1483.3 | 29 | 0.47 | 4cbl | 1332.7 | 6 | 0.20 |
| 4ju5 | 1810.7 | 214 | 0.97 | 4cbm | 1180.1 | 0 | 0.12 |
| 4jup | 389.5 | 20 | 0.38 | 4cdo | 458.8 | 20 | 0.38 |
| 4k2e | 1349.0 | 163 | 0.84 | 4cfi | 628.2 | 0 | 0.12 |
| 4kde | 1615.9 | 281 | 1.00 | 4ch7 | 579.2 | 0 | 0.12 |
| 4ke2 | 1787.5 | 4 | 0.18 | 4chj | 930.5 | 144 | 0.83 |
| 4km3 | 1157.9 | 125 | 0.83 | 4cil | 783.5 | 2 | 0.15 |
| 4kn8 | 1201.8 | 255 | 1.00 | 4co7 | 515.3 | 0 | 0.12 |
| 4kp2 | 1756.8 | 41 | 0.57 | 4cso | 1146.4 | 5 | 0.19 |
| 4kz1 | 695.3 | 104 | 0.81 | 4cx8 | 746.1 | 0 | 0.12 |
| 4l2w | 1072.2 | 47 | 0.61 | 4cxi | 2001.1 | 145 | 0.83 |
| 4l4q | 2598.3 | 74 | 0.74 | 4cye | 684.5 | 148 | 0.83 |
| 4l69 | 1287.4 | 132 | 0.83 | 4d2o | 1026.0 | 0 | 0.12 |
| 4l9e | 1306.0 | 391 | 1.00 | 4d4q | 533.7 | 0 | 0.12 |
| 4le5 | 2448.8 | 46 | 0.60 | 4d5r | 790.3 | 109 | 0.81 |
| 4lft | 517.9 | 0 | 0.12 | 4d70 | 445.7 | 0 | 0.12 |
| 4ljk | 791.5 | 194 | 0.89 | 4d7r | 523.9 | 0 | 0.12 |
| 4ljl | 710.3 | 213 | 0.96 | 4h9w | 438.6 | 2 | 0.15 |
| 4lpu | 2061.2 | 98 | 0.80 | 4hic | 542.7 | 0 | 0.12 |
| 4lpw | 1916.8 | 74 | 0.74 | 4icu | 545.8 | 0 | 0.12 |
| 4lpx | 2109.4 | 50 | 0.63 | 4ino | 904.8 | 0 | 0.12 |
| 4ltb | 5267.9 | 18 | 0.35 | 4iqc | 581.3 | 1 | 0.13 |
| 4luy | 3263.7 | 115 | 0.82 | 4irf | 674.0 | 22 | 0.40 |
| 4lwo | 1645.7 | 102 | 0.81 | 4it7 | 466.5 | 0 | 0.12 |
| 4m0d | 4320.9 | 55 | 0.66 | 4iyc | 773.1 | 0 | 0.12 |
| 4m0q | 1449.4 | 83 | 0.77 | 4ize | 764.7 | 13 | 0.29 |
| 4m23 | 1547.5 | 86 | 0.78 | 4izl | 772.1 | 0 | 0.12 |
| 4m36 | 3405.2 | 47 | 0.61 | 4j0o | 798.6 | 0 | 0.12 |
| 4m6a | 2105.6 | 117 | 0.82 | 4j1s | 602.8 | 3 | 0.16 |
| 4m8z | 965.3 | 103 | 0.81 | 4j2r | 620.9 | 0 | 0.12 |
| 4mac | 488.9 | 106 | 0.81 | 4jkq | 787.4 | 0 | 0.12 |
| 4mdu | 943.7 | 5 | 0.19 | 4jmp | 454.7 | 0 | 0.12 |
| 4mea | 1505.2 | 351 | 1.00 | 4k1s | 473.8 | 0 | 0.12 |
| 4mei | 682.9 | 14 | 0.31 | 4k40 | 692.2 | 0 | 0.12 |
| 4mfu | 963.5 | 0 | 0.12 | 4k51 | 874.1 | 0 | 0.12 |
| 4mfv | 896.3 | 0 | 0.12 | 4k5q | 626.7 | 0 | 0.12 |
| 4mid | 1266.1 | 192 | 0.89 | 4k82 | 729.0 | 0 | 0.12 |
| 4mir | 1560.6 | 187 | 0.87 | 4k83 | 565.0 | 39 | 0.55 |
| 4mis | 1493.7 | 206 | 0.93 | 4k9s | 727.3 | 0 | 0.12 |
| 4ml3 | 811.0 | 52 | 0.64 | 4kex | 449.1 | 0 | 0.12 |
| 4mld | 758.2 | 57 | 0.67 | 4kxo | 1758.6 | 186 | 0.87 |
| 4mmn | 831.4 | 311 | 1.00 | 4l1d | 447.5 | 25 | 0.43 |
| 4mpl | 1249.3 | 144 | 0.83 | 4l6u | 635.4 | 0 | 0.12 |
| 4mt8 | 2024.5 | 47 | 0.61 | 4l8i | 827.8 | 0 | 0.12 |
| 4mtx | 2122.5 | 44 | 0.59 | 4l8l | 871.1 | 141 | 0.83 |
| 4muo | 1129.0 | 109 | 0.81 | 4l9h | 1109.1 | 85 | 0.78 |
| 4mxm | 1122.6 | 130 | 0.83 | 4lcm | 814.0 | 0 | 0.12 |
| 4myc | 6853.3 | 10 | 0.26 | 4lee | 564.5 | 0 | 0.12 |
| 4myz | 1566.4 | 402 | 1.00 | 4lhf | 1034.8 | 148 | 0.83 |
| 4mzm | 1257.7 | 246 | 1.00 | 4lk4 | 595.0 | 9 | 0.24 |
| 4mzp | 1277.0 | 219 | 0.99 | 4lpt | 788.0 | 40 | 0.56 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4mzt | 1239.1 | 182 | 0.86 | 4lrk | 1351.9 | 126 | 0.83 |
| 4n06 | 1254.8 | 56 | 0.66 | 4lso | 524.0 | 0 | 0.12 |
| 4n1k | 871.5 | 22 | 0.40 | 4ltt | 406.7 | 0 | 0.12 |
| 4n1y | 1624.5 | 185 | 0.87 | 4lw5 | 681.9 | 1 | 0.13 |
| 4n92 | 584.4 | 0 | 0.12 | 4lzi | 660.2 | 64 | 0.70 |
| 4n9h | 1857.9 | 155 | 0.84 | 4m64 | 828.6 | 0 | 0.12 |
| 4na2 | 2607.9 | 78 | 0.76 | 4m7g | 499.9 | 0 | 0.12 |
| 4ncd | 855.9 | 151 | 0.83 | 4m80 | 602.7 | 0 | 0.12 |
| 4ndj | 2363.8 | 70 | 0.73 | 4m8g | 577.1 | 20 | 0.38 |
| 4ndk | 1414.9 | 151 | 0.83 | 4m90 | 630.5 | 0 | 0.12 |
| 4ndw | 2010.2 | 199 | 0.91 | 4m9p | 903.2 | 17 | 0.34 |
| 4nj0 | 882.7 | 229 | 1.00 | 4mc0 | 641.1 | 0 | 0.12 |
| 4nj1 | 924.9 | 217 | 0.98 | 4mck | 1005.3 | 26 | 0.44 |
| 4nk7 | 785.6 | 45 | 0.60 | 4mee | 423.1 | 0 | 0.12 |
| 4nkk | 1467.8 | 331 | 1.00 | 4mel | 1516.8 | 187 | 0.87 |
| 4nn1 | 3044.8 | 243 | 1.00 | 4mem | 992.7 | 24 | 0.42 |
| 4nom | 813.5 | 0 | 0.12 | 4mfi | 957.9 | 20 | 0.38 |
| 4npu | 1565.1 | 382 | 1.00 | 4mfj | 742.9 | 1 | 0.13 |
| 4nqf | 1203.6 | 32 | 0.49 | 4mgf | 1031.0 | 27 | 0.45 |
| 4nqt | 1286.7 | 67 | 0.72 | 4mgs | 415.5 | 0 | 0.12 |
| 4nsr | 1126.8 | 138 | 0.83 | 4mhp | 712.7 | 0 | 0.12 |
| 4nsw | 5938.3 | 14 | 0.31 | 4mhr | 1037.8 | 260 | 1.00 |
| 4ny0 | 735.5 | 0 | 0.12 | 4mq3 | 525.1 | 0 | 0.12 |
| 4o0q | 1498.6 | 237 | 1.00 | 4mt5 | 743.5 | 9 | 0.24 |
| 4o1h | 731.2 | 319 | 1.00 | 4mt6 | 713.4 | 0 | 0.12 |
| 4o2h | 919.3 | 20 | 0.38 | 4mt7 | 458.5 | 0 | 0.12 |
| 4o60 | 1437.3 | 1 | 0.13 | 4mzd | 399.1 | 0 | 0.12 |
| 4o8b | 1438.0 | 274 | 1.00 | 4n08 | 683.6 | 0 | 0.12 |
| 4oaf | 1130.5 | 28 | 0.46 | 4n1l | 691.4 | 9 | 0.24 |
| 4oft | 1298.0 | 255 | 1.00 | 4n3x | 940.2 | 122 | 0.82 |
| 4ogd | 2516.7 | 71 | 0.73 | 4n40 | 654.7 | 0 | 0.12 |
| 4ogf | 1330.1 | 149 | 0.83 | 4n4a | 1357.1 | 5 | 0.19 |
| 4oh9 | 1447.5 | 132 | 0.83 | 4n5a | 856.9 | 0 | 0.12 |
| 4oi3 | 1069.6 | 416 | 1.00 | 4n5c | 944.0 | 0 | 0.12 |
| 4okc | 2395.3 | 129 | 0.83 | 4n5q | 877.0 | 2 | 0.15 |
| 4oky | 811.4 | 26 | 0.44 | 4n6l | 796.5 | 6 | 0.20 |
| 4om7 | 671.5 | 32 | 0.49 | 4n6t | 555.7 | 0 | 0.12 |
| 4omt | 1234.1 | 12 | 0.28 | 4n6u | 591.8 | 0 | 0.12 |
| 4ooi | 1425.5 | 219 | 0.99 | 4n75 | 486.6 | 0 | 0.12 |
| 4or8 | 3048.9 | 108 | 0.81 | 4n7f | 626.1 | 142 | 0.83 |
| 4otm | 2117.8 | 137 | 0.83 | 4n8h | 1844.3 | 36 | 0.53 |
| 4oun | 1301.0 | 168 | 0.85 | 4n8k | 1885.0 | 42 | 0.58 |
| 4p08 | 1192.2 | 39 | 0.55 | 4n8l | 1813.1 | 30 | 0.48 |
| 4p12 | 1514.5 | 37 | 0.54 | 4nbo | 626.7 | 36 | 0.53 |
| 4p22 | 2447.4 | 55 | 0.66 | 4nc9 | 920.1 | 25 | 0.43 |
| 4p61 | 1613.3 | 276 | 1.00 | 4nci | 594.3 | 53 | 0.65 |
| 4p6k | 544.4 | 8 | 0.23 | 4ndl | 376.7 | 0 | 0.12 |
| 4p6l | 535.0 | 1 | 0.13 | 4nfb | 772.8 | 0 | 0.12 |
| 4p96 | 1702.6 | 97 | 0.80 | 4nfc | 641.8 | 33 | 0.50 |
| 4p9f | 1175.1 | 105 | 0.81 | 4nfx | 1640.6 | 226 | 1.00 |
| 4pd0 | 3058.9 | 40 | 0.56 | 4ng0 | 407.9 | 382 | 1.00 |
| 4pdp | 738.4 | 0 | 0.12 | 4nj6 | 657.2 | 57 | 0.67 |
| 4pgg | 4733.5 | 121 | 0.82 | 4nj7 | 462.7 | 0 | 0.12 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4ph6 | 990.4 | 145 | 0.83 | 4nj8 | 364.8 | 0 | 0.12 |
| 4pmu | 955.2 | 117 | 0.82 | 4njc | 726.7 | 368 | 1.00 |
| 4pn0 | 2112.5 | 172 | 0.85 | 4nk6 | 807.5 | 17 | 0.34 |
| 4pon | 1508.6 | 226 | 1.00 | 4nk8 | 803.6 | 84 | 0.77 |
| 4prs | 1471.2 | 120 | 0.82 | 4nl7 | 1254.8 | 0 | 0.12 |
| 4pu7 | 1034.3 | 282 | 1.00 | 4nlb | 611.1 | 0 | 0.12 |
| 4pu8 | 1047.0 | 229 | 1.00 | 4nng | 613.8 | 0 | 0.12 |
| 4puh | 705.7 | 327 | 1.00 | 4nnh | 602.0 | 11 | 0.27 |
| 4pus | 653.0 | 0 | 0.12 | 4nnk | 673.3 | 0 | 0.12 |
| 4pvc | 1038.6 | 97 | 0.80 | 4noj | 473.9 | 0 | 0.12 |
| 4pz9 | 792.6 | 15 | 0.32 | 4npf | 1404.4 | 182 | 0.86 |
| 4pzc | 1882.4 | 201 | 0.91 | 4nq0 | 624.3 | 0 | 0.12 |
| 4q0c | 4048.2 | 69 | 0.73 | 4nsp | 695.8 | 0 | 0.12 |
| 4q20 | 1582.8 | 106 | 0.81 | 4nu2 | 651.3 | 0 | 0.12 |
| 4q25 | 1306.1 | 54 | 0.65 | 4nv8 | 837.6 | 73 | 0.74 |
| 4q2o | 1481.0 | 282 | 1.00 | 4nx9 | 1116.7 | 58 | 0.68 |
| 4q2q | 1345.1 | 420 | 1.00 | 4nzz | 497.2 | 0 | 0.12 |
| 4q75 | 3807.5 | 100 | 0.80 | 4o2x | 524.9 | 15 | 0.32 |
| 4q76 | 3645.9 | 100 | 0.80 | 4o3x | 376.2 | 0 | 0.12 |
| 4q97 | 977.5 | 26 | 0.44 | 4o4c | 814.6 | 23 | 0.41 |
| 4q9b | 727.8 | 140 | 0.83 | 4o5p | 352.7 | 0 | 0.12 |
| 4qfb | 656.8 | 0 | 0.12 | 4o5s | 382.7 | 0 | 0.12 |
| 4qhr | 2359.5 | 137 | 0.83 | 4o6g | 579.5 | 1 | 0.13 |
| 4qjn | 1902.4 | 166 | 0.84 | 4o6k | 880.3 | 6 | 0.20 |
| 4ql6 | 1293.0 | 0 | 0.12 | 4o6x | 616.0 | 151 | 0.83 |
| 4qr0 | 1428.3 | 229 | 1.00 | 4o7q | 357.0 | 0 | 0.12 |
| 4qr1 | 1396.3 | 235 | 1.00 | 4o8s | 340.7 | 1 | 0.13 |
| 4qr2 | 1398.5 | 230 | 1.00 | 4o8v | 613.5 | 0 | 0.12 |
| 4qva | 1921.1 | 15 | 0.32 | 4o9f | 621.2 | 0 | 0.12 |
| 4qvg | 3542.2 | 190 | 0.88 | 4o9l | 660.7 | 5 | 0.19 |
| 4qvj | 1923.1 | 15 | 0.32 | 4oa6 | 410.0 | 0 | 0.12 |
| 4qxz | 689.0 | 117 | 0.82 | 4ob4 | 577.0 | 64 | 0.70 |
| 4qyx | 532.0 | 7 | 0.22 | 4od4 | 650.6 | 0 | 0.12 |
| 4r0b | 1180.1 | 97 | 0.80 | 4od6 | 423.7 | 0 | 0.12 |
| 4r1i | 1813.7 | 12 | 0.28 | 4odd | 638.8 | 78 | 0.76 |
| 4r1n | 1837.7 | 254 | 1.00 | 4of0 | 898.4 | 0 | 0.12 |
| 4r27 | 890.3 | 0 | 0.12 | 4of5 | 565.9 | 0 | 0.12 |
| 4r3q | 2250.6 | 94 | 0.79 | 4ofv | 574.2 | 0 | 0.12 |
| 4r8e | 2890.5 | 89 | 0.79 | 4ohd | 1073.1 | 0 | 0.12 |
| 4ra8 | 670.7 | 2 | 0.15 | 4ohe | 788.4 | 0 | 0.12 |
| 4rct | 1569.6 | 96 | 0.80 | 4ohh | 873.1 | 0 | 0.12 |
| 4rd9 | 1799.3 | 77 | 0.75 | 4ohi | 825.7 | 0 | 0.12 |
| 4rdj | 1762.0 | 90 | 0.79 | 4ohl | 652.1 | 0 | 0.12 |
| 4rg7 | 2210.3 | 199 | 0.91 | 4ohr | 1356.2 | 306 | 1.00 |
| 4rie | 1498.0 | 76 | 0.75 | 4oj0 | 1524.5 | 139 | 0.83 |
| 4rmb | 2540.6 | 211 | 0.95 | 4ok0 | 290.2 | 0 | 0.12 |
| 4rni | 1077.7 | 29 | 0.47 | 4om9 | 794.9 | 0 | 0.12 |
| 4rnj | 772.9 | 14 | 0.31 | 4oq1 | 1078.4 | 0 | 0.12 |
| 4rns | 2014.2 | 191 | 0.88 | 4oqw | 1470.9 | 225 | 1.00 |
| 4rsj | 2314.0 | 33 | 0.50 | 4orw | 520.5 | 0 | 0.12 |
| 4rsw | 1615.5 | 34 | 0.51 | 4os0 | 1024.8 | 452 | 1.00 |
| 4rvs | 1189.0 | 49 | 0.62 | 4os3 | 1046.9 | 333 | 1.00 |
| 4ry2 | 5221.6 | 20 | 0.38 | 4os8 | 1010.5 | 369 | 1.00 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4ryj | 476.7 | 0 | 0.12 | 4otd | 731.8 | 0 | 0.12 |
| 4ryp | 3238.5 | 111 | 0.82 | 4ou0 | 280.0 | 7 | 0.22 |
| 4s03 | 851.7 | 49 | 0.62 | 4ow6 | 482.5 | 0 | 0.12 |
| 4s0j | 849.4 | 50 | 0.63 | 4oyl | 381.5 | 0 | 0.12 |
| 4to7 | 1040.6 | 340 | 1.00 | 4oyy | 539.1 | 0 | 0.12 |
| 4tq7 | 774.9 | 108 | 0.81 | 4ozk | 393.0 | 0 | 0.12 |
| 4tqj | 949.5 | 305 | 1.00 | 4p09 | 778.0 | 0 | 0.12 |
| 4tr7 | 1139.1 | 28 | 0.46 | 4p0f | 1184.7 | 19 | 0.36 |
| 4trh | 2343.9 | 16 | 0.33 | 4p0j | 758.0 | 50 | 0.63 |
| 4trt | 1084.6 | 26 | 0.44 | 4p0k | 730.5 | 94 | 0.79 |
| 4ttw | 624.3 | 0 | 0.12 | 4p0l | 748.4 | 6 | 0.20 |
| 4ttx | 826.7 | 283 | 1.00 | 4p0m | 844.4 | 5 | 0.19 |
| 4u2i | 913.8 | 420 | 1.00 | 4p0o | 1113.1 | 23 | 0.41 |
| 4u2u | 3170.2 | 65 | 0.71 | 4p0y | 485.3 | 0 | 0.12 |
| 4u3q | 651.0 | 0 | 0.12 | 4p0z | 476.1 | 0 | 0.12 |
| 4u4i | 925.8 | 11 | 0.27 | 4p17 | 755.8 | 1 | 0.13 |
| 4u5h | 590.7 | 11 | 0.27 | 4p39 | 783.3 | 22 | 0.40 |
| 4u64 | 1516.7 | 129 | 0.83 | 4p47 | 730.3 | 0 | 0.12 |
| 4u9c | 430.5 | 0 | 0.12 | 4p48 | 312.2 | 0 | 0.12 |
| 4ua2 | 1791.7 | 77 | 0.75 | 4p5u | 575.6 | 0 | 0.12 |
| 4uds | 2686.6 | 183 | 0.87 | 4p7o | 1213.8 | 3 | 0.16 |
| 4up8 | 4485.2 | 82 | 0.77 | 4pa1 | 1179.0 | 57 | 0.67 |
| 4uu3 | 1420.2 | 178 | 0.86 | 4pbd | 917.9 | 43 | 0.58 |
| 4uvj | 1053.6 | 13 | 0.29 | 4pcf | 657.7 | 0 | 0.12 |
| 4uzn | 550.4 | 0 | 0.12 | 4pd3 | 1330.8 | 8 | 0.23 |
| 4v1p | 637.6 | 187 | 0.87 | 4pej | 1102.3 | 46 | 0.60 |
| 4v2f | 2260.3 | 121 | 0.82 | 4pek | 665.9 | 0 | 0.12 |
| 4w4r | 996.8 | 34 | 0.51 | 4pgr | 605.0 | 0 | 0.12 |
| 4w69 | 859.5 | 57 | 0.67 | 4pgs | 644.6 | 0 | 0.12 |
| 4w6a | 721.1 | 126 | 0.83 | 4pgu | 550.2 | 2 | 0.15 |
| 4w6c | 921.9 | 79 | 0.76 | 4pgv | 572.7 | 1 | 0.13 |
| 4w6g | 903.5 | 138 | 0.83 | 4ph1 | 682.9 | 70 | 0.73 |
| 4w6h | 714.0 | 69 | 0.73 | 4pjq | 697.2 | 6 | 0.20 |
| 4w6i | 675.5 | 110 | 0.82 | 4pk1 | 480.4 | 0 | 0.12 |
| 4w6k | 770.7 | 78 | 0.76 | 4pk9 | 2832.5 | 86 | 0.78 |
| 4w6l | 959.2 | 18 | 0.35 | 4pka | 2944.0 | 109 | 0.81 |
| 4w6n | 817.4 | 67 | 0.72 | 4pkx | 510.9 | 0 | 0.12 |
| 4w6o | 754.8 | 119 | 0.82 | 4pmh | 582.2 | 0 | 0.12 |
| 4w6p | 915.5 | 57 | 0.67 | 4pn7 | 702.5 | 0 | 0.12 |
| 4w6r | 835.5 | 93 | 0.79 | 4po4 | 622.8 | 0 | 0.12 |
| 4w7x | 819.9 | 83 | 0.77 | 4poy | 441.2 | 0 | 0.12 |
| 4w8i | 3009.0 | 87 | 0.78 | 4ppj | 977.6 | 0 | 0.12 |
| 4wd9 | 3030.4 | 47 | 0.61 | 4ppk | 921.5 | 0 | 0.12 |
| 4whj | 1018.7 | 56 | 0.66 | 4ppl | 1001.2 | 0 | 0.12 |
| 4wic | 2466.7 | 17 | 0.34 | 4pqo | 488.6 | 0 | 0.12 |
| 4wij | 4371.7 | 26 | 0.44 | 4pqz | 377.1 | 0 | 0.12 |
| 4wik | 4164.8 | 28 | 0.46 | 4psd | 472.6 | 0 | 0.12 |
| 4wja | 1393.0 | 369 | 1.00 | 4psf | 595.2 | 8 | 0.23 |
| 4wnz | 1286.8 | 53 | 0.65 | 4pug | 826.8 | 0 | 0.12 |
| 4wo7 | 1830.4 | 241 | 1.00 | 4pui | 476.4 | 0 | 0.12 |
| 4wpe | 3979.6 | 51 | 0.64 | 4pwq | 802.1 | 1 | 0.13 |
| 4wse | 3250.3 | 45 | 0.60 | 4pzp | 538.0 | 0 | 0.12 |
| 4wt5 | 1363.3 | 109 | 0.81 | 4q2s | 467.6 | 0 | 0.12 |

| | | | |
|---|---|---|---|
| 4wum | 2951.4 | 86 | 0.78 |
| 4wy8 | 1280.4 | 75 | 0.75 |
| 4x0r | 1026.9 | 168 | 0.85 |
| 4x5n | 1515.3 | 43 | 0.58 |
| 4x5u | 3721.3 | 34 | 0.51 |
| 4x8f | 1205.5 | 354 | 1.00 |
| 4xa1 | 3974.0 | 11 | 0.27 |
| 4xa3 | 3674.4 | 13 | 0.29 |
| 4xa4 | 2472.8 | 24 | 0.42 |
| 4xa6 | 4370.0 | 9 | 0.24 |
| 4xbx | 1614.6 | 202 | 0.92 |
| 4xlx | 1062.3 | 77 | 0.75 |
| 4xo1 | 1576.0 | 209 | 0.94 |
| 4xo2 | 1581.3 | 220 | 1.00 |
| 4xoh | 1083.9 | 6 | 0.20 |
| 4xws | 1050.8 | 49 | 0.62 |
| 4xyg | 3638.3 | 188 | 0.88 |
| 4xz7 | 2973.9 | 89 | 0.79 |
| 4y0m | 1294.5 | 92 | 0.79 |
| 4y9a | 1662.8 | 218 | 0.99 |
| 4ylt | 1916.7 | 186 | 0.87 |
| 4ymr | 2237.6 | 80 | 0.76 |
| 4ynh | 1528.6 | 297 | 1.00 |
| 4yub | 2778.3 | 74 | 0.74 |
| 4yzy | 1008.9 | 39 | 0.55 |
| 4z27 | 1546.0 | 99 | 0.80 |
| 4z6j | 1571.1 | 157 | 0.84 |
| 4zbh | 510.6 | 171 | 0.85 |
| 4zbw | 472.6 | 0 | 0.12 |
| 4zm8 | 3174.8 | 43 | 0.58 |
| 4zqa | 1794.3 | 58 | 0.68 |
| 5a0o | 974.7 | 0 | 0.12 |
| 5a2n | 1096.1 | 0 | 0.12 |
| 5a48 | 778.2 | 1 | 0.13 |
| 5bto | 876.8 | 22 | 0.40 |

| | | | |
|---|---|---|---|
| 4q2y | 1153.2 | 8 | 0.23 |
| 4q3h | 460.7 | 172 | 0.85 |
| 4q4g | 422.2 | 0 | 0.12 |
| 4q4n | 425.5 | 0 | 0.12 |
| 4q5y | 1028.2 | 8 | 0.23 |
| 4q65 | 58.7 | 0 | 0.12 |
| 4q6l | 600.1 | 0 | 0.12 |
| 4q6v | 559.9 | 0 | 0.12 |
| 4q6z | 625.4 | 0 | 0.12 |
| 4q7k | 355.4 | 0 | 0.12 |
| 4q7m | 1390.7 | 166 | 0.84 |
| 4q7t | 528.1 | 0 | 0.12 |
| 4q9h | 661.2 | 0 | 0.12 |
| 4q9p | 775.3 | 58 | 0.68 |
| 4qaj | 584.1 | 46 | 0.60 |
| 4qaz | 634.2 | 1 | 0.13 |
| 4qb0 | 467.1 | 0 | 0.12 |
| 4qbe | 634.5 | 25 | 0.43 |
| 4qcj | 472.0 | 14 | 0.31 |
| 4qdr | 682.2 | 0 | 0.12 |
| 4qdt | 562.9 | 0 | 0.12 |
| 4qdu | 659.9 | 0 | 0.12 |
| 4qgy | 573.2 | 0 | 0.12 |
| 4qlo | 1517.2 | 96 | 0.80 |
| 4qlr | 618.0 | 2 | 0.15 |
| 4qmd | 653.3 | 0 | 0.12 |
| 4qmi | 856.6 | 0 | 0.12 |
| 4qmj | 902.9 | 0 | 0.12 |
| 4qs8 | 630.1 | 0 | 0.12 |
| 4qt4 | 599.0 | 0 | 0.12 |
| 4qtz | 630.7 | 0 | 0.12 |
| 4quc | 200.4 | 0 | 0.12 |
| 4quk | 419.9 | 0 | 0.12 |
| 4qx0 | 1356.7 | 12 | 0.28 |
| 4qx1 | 1328.2 | 6 | 0.20 |
| 4qx2 | 1335.0 | 11 | 0.27 |
| 4qx3 | 1326.8 | 9 | 0.24 |
| 4qxl | 385.4 | 0 | 0.12 |
| 4r05 | 588.3 | 0 | 0.12 |
| 4r0e | 452.6 | 30 | 0.48 |
| 4r0x | 671.7 | 0 | 0.12 |
| 4r0y | 793.2 | 0 | 0.12 |
| 4r19 | 706.5 | 0 | 0.12 |
| 4r1a | 468.7 | 0 | 0.12 |
| 4r1b | 536.5 | 0 | 0.12 |
| 4r1c | 549.8 | 0 | 0.12 |
| 4r58 | 574.3 | 0 | 0.12 |
| 4r61 | 710.9 | 31 | 0.49 |
| 4r6f | 782.0 | 0 | 0.12 |
| 4r7v | 757.5 | 4 | 0.18 |
| 4r8r | 680.7 | 0 | 0.12 |
| 4rcw | 1336.8 | 22 | 0.40 |
| 4rdp | 1381.7 | 111 | 0.82 |

| | | | |
|---|---|---|---|
| 4reh | 643.8 | 0 | 0.12 |
| 4rej | 614.6 | 0 | 0.12 |
| 4rf6 | 896.8 | 0 | 0.12 |
| 4rid | 1471.5 | 4 | 0.18 |
| 4rl1 | 661.6 | 0 | 0.12 |
| 4rl9 | 506.7 | 0 | 0.12 |
| 4rlb | 816.1 | 0 | 0.12 |
| 4rlm | 560.4 | 0 | 0.12 |
| 4rln | 568.5 | 0 | 0.12 |
| 4ro1 | 226.8 | 0 | 0.12 |
| 4roa | 729.3 | 27 | 0.45 |
| 4rs6 | 869.0 | 122 | 0.82 |
| 4rsq | 767.9 | 28 | 0.46 |
| 4rsx | 933.4 | 0 | 0.12 |
| 4rtd | 1339.0 | 1 | 0.13 |
| 4rth | 1038.2 | 32 | 0.49 |
| 4rwi | 1184.5 | 55 | 0.66 |
| 4rwq | 645.6 | 0 | 0.12 |
| 4rwr | 1023.5 | 86 | 0.78 |
| 4rwu | 734.0 | 46 | 0.60 |
| 4rwz | 895.4 | 91 | 0.79 |
| 4ry4 | 939.0 | 0 | 0.12 |
| 4ry6 | 963.0 | 0 | 0.12 |
| 4ry7 | 958.1 | 0 | 0.12 |
| 4rz2 | 769.4 | 0 | 0.12 |
| 4s11 | 565.3 | 0 | 0.12 |
| 4s3l | 495.4 | 2 | 0.15 |
| 4s3p | 2064.0 | 46 | 0.60 |
| 4tks | 1025.6 | 43 | 0.58 |
| 4tlp | 587.8 | 0 | 0.12 |
| 4tlw | 863.4 | 0 | 0.12 |
| 4tn9 | 489.6 | 0 | 0.12 |
| 4tnm | 642.4 | 0 | 0.12 |
| 4tql | 785.7 | 0 | 0.12 |
| 4tr5 | 1340.3 | 222 | 1.00 |
| 4trk | 536.2 | 0 | 0.12 |
| 4tse | 1057.9 | 26 | 0.44 |
| 4ttl | 125.0 | 0 | 0.12 |
| 4ttp | 530.3 | 0 | 0.12 |
| 4tum | 515.8 | 11 | 0.27 |
| 4tut | 161.3 | 96 | 0.80 |
| 4tuu | 517.7 | 0 | 0.12 |
| 4tve | 480.4 | 2 | 0.15 |
| 4tx2 | 695.4 | 0 | 0.12 |
| 4txp | 464.4 | 0 | 0.12 |
| 4tza | 906.5 | 9 | 0.24 |
| 4tzg | 1452.9 | 96 | 0.80 |
| 4tzi | 605.0 | 0 | 0.12 |
| 4tzj | 640.7 | 0 | 0.12 |
| 4u0l | 753.8 | 0 | 0.12 |
| 4u1d | 1336.3 | 3 | 0.16 |
| 4u2m | 664.7 | 17 | 0.34 |
| 4u2n | 698.3 | 224 | 1.00 |

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|---|---|---|---|
| 4u3a | 1320.8 | 202 | 0.92 |
| 4u3h | 795.9 | 0 | 0.12 |
| 4u3t | 871.0 | 2 | 0.15 |
| 4u3v | 631.7 | 0 | 0.12 |
| 4u48 | 4122.1 | 21 | 0.39 |
| 4u4h | 1423.8 | 1 | 0.13 |
| 4u4j | 4204.9 | 24 | 0.42 |
| 4u59 | 4234.2 | 24 | 0.42 |
| 4u5a | 629.0 | 0 | 0.12 |
| 4u9q | 724.9 | 28 | 0.46 |
| 4ud5 | 886.9 | 0 | 0.12 |
| 4uex | 709.7 | 0 | 0.12 |
| 4ulw | 859.8 | 132 | 0.83 |
| 4umg | 601.3 | 9 | 0.24 |
| 4ums | 460.4 | 6 | 0.20 |
| 4uos | 526.4 | 22 | 0.40 |
| 4uts | 752.4 | 0 | 0.12 |
| 4uu4 | 881.4 | 17 | 0.34 |
| 4uv2 | 1979.0 | 80 | 0.76 |
| 4uv6 | 799.7 | 72 | 0.74 |
| 4uvk | 744.7 | 0 | 0.12 |
| 4uw2 | 1029.0 | 0 | 0.12 |
| 4uww | 441.0 | 250 | 1.00 |
| 4uy3 | 418.9 | 0 | 0.12 |
| 4uz2 | 739.0 | 5 | 0.19 |
| 4v0t | 978.3 | 152 | 0.83 |
| 4v14 | 423.1 | 0 | 0.12 |
| 4v16 | 789.0 | 0 | 0.12 |
| 4v2b | 539.8 | 0 | 0.12 |
| 4v2d | 696.1 | 0 | 0.12 |
| 4v2e | 1539.3 | 0 | 0.12 |
| 4v2u | 357.2 | 0 | 0.12 |
| 4v38 | 372.1 | 0 | 0.12 |
| 4v39 | 359.2 | 0 | 0.12 |
| 4w4m | 595.1 | 0 | 0.12 |
| 4w5x | 437.2 | 18 | 0.35 |
| 4w60 | 399.3 | 37 | 0.54 |
| 4w6v | 673.6 | 0 | 0.12 |
| 4w7g | 525.1 | 0 | 0.12 |
| 4w8v | 2072.4 | 302 | 1.00 |
| 4w8w | 1381.4 | 116 | 0.82 |
| 4w8z | 1533.3 | 143 | 0.83 |
| 4wau | 818.2 | 16 | 0.33 |
| 4wbz | 673.2 | 22 | 0.40 |
| 4wdc | 428.5 | 0 | 0.12 |
| 4we2 | 291.9 | 0 | 0.12 |
| 4wfi | 551.9 | 0 | 0.12 |
| 4wj1 | 1240.1 | 33 | 0.50 |
| 4wj2 | 595.3 | 0 | 0.12 |
| 4wjs | 491.1 | 0 | 0.12 |
| 4wmg | 599.5 | 0 | 0.12 |
| 4wo8 | 844.0 | 0 | 0.12 |
| 4woy | 1029.5 | 44 | 0.59 |

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|---|---|---|---|
| 4wp6 | 558.9 | 0 | 0.12 |
| 4wt3 | 425.1 | 0 | 0.12 |
| 4wtx | 501.6 | 3 | 0.16 |
| 4wu0 | 868.2 | 11 | 0.27 |
| 4wz0 | 701.2 | 48 | 0.62 |
| 4x0j | 912.8 | 0 | 0.12 |
| 4x2m | 562.7 | 0 | 0.12 |
| 4x2w | 1095.6 | 44 | 0.59 |
| 4x2x | 580.8 | 4 | 0.18 |
| 4x2y | 805.9 | 38 | 0.54 |
| 4x3x | 712.4 | 0 | 0.12 |
| 4x43 | 643.0 | 0 | 0.12 |
| 4x8h | 974.2 | 6 | 0.20 |
| 4x8m | 978.8 | 0 | 0.12 |
| 4x9u | 375.5 | 0 | 0.12 |
| 4xah | 703.5 | 311 | 1.00 |
| 4xeh | 5944.1 | 35 | 0.52 |
| 4xfu | 599.9 | 0 | 0.12 |
| 4xfv | 758.8 | 0 | 0.12 |
| 4xh3 | 767.8 | 0 | 0.12 |
| 4xhm | 554.3 | 3 | 0.16 |
| 4xkk | 495.8 | 1 | 0.13 |
| 4xm4 | 1840.7 | 79 | 0.76 |
| 4xp8 | 487.4 | 17 | 0.34 |
| 4xpk | 578.7 | 0 | 0.12 |
| 4xq7 | 607.0 | 0 | 0.12 |
| 4xy3 | 578.5 | 0 | 0.12 |
| 4xzg | 666.3 | 0 | 0.12 |
| 4y21 | 1200.0 | 28 | 0.46 |
| 4y4q | 858.6 | 9 | 0.24 |
| 4y5j | 1107.5 | 16 | 0.33 |
| 4yeq | 874.7 | 17 | 0.34 |
| 4yf2 | 735.9 | 0 | 0.12 |
| 4yfe | 383.1 | 0 | 0.12 |
| 4yfs | 692.9 | 0 | 0.12 |
| 4yhe | 555.5 | 0 | 0.12 |
| 4ykc | 961.7 | 22 | 0.40 |
| 4ykd | 532.1 | 0 | 0.12 |
| 4yno | 880.1 | 0 | 0.12 |
| 4ynv | 644.0 | 203 | 0.92 |
| 4ynw | 651.0 | 246 | 1.00 |
| 4ypj | 838.6 | 0 | 0.12 |
| 4yuo | 353.0 | 0 | 0.12 |
| 4yvm | 1688.5 | 20 | 0.38 |
| 4yvo | 482.7 | 0 | 0.12 |
| 4z29 | 938.1 | 29 | 0.47 |
| 4z99 | 583.3 | 0 | 0.12 |
| 4z9p | 781.4 | 67 | 0.72 |
| 4zf3 | 739.3 | 15 | 0.32 |
| 4zf4 | 587.1 | 22 | 0.40 |
| 4zf5 | 749.1 | 38 | 0.54 |
| 4zg1 | 539.5 | 0 | 0.12 |
| 4zj2 | 454.2 | 0 | 0.12 |

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|---|---|---|---|---|---|---|---|
| | | | | 4zj3 | 404.1 | 0 | 0.12 |
| | | | | 4zmd | 382.5 | 0 | 0.12 |
| | | | | 4zot | 532.0 | 0 | 0.12 |
| | | | | 4zov | 1138.3 | 158 | 0.84 |
| | | | | 4zoy | 734.9 | 0 | 0.12 |
| | | | | 4zuz | 1005.3 | 5 | 0.19 |
| | | | | 4zwj | 1081.6 | 0 | 0.12 |
| | | | | 5a0g | 720.4 | 0 | 0.12 |
| | | | | 5a0z | 1330.2 | 37 | 0.54 |
| | | | | 5aem | 898.4 | 4 | 0.18 |
| | | | | 5af5 | 291.9 | 0 | 0.12 |
| | | | | 5aio | 872.5 | 104 | 0.81 |
| | | | | 5aj8 | 671.6 | 0 | 0.12 |
| | | | | 5avg | 710.4 | 13 | 0.29 |
| | | | | 5avh | 4608.7 | 89 | 0.79 |
| | | | | 5brl | 535.8 | 5 | 0.19 |
| | | | | 5bth | 695.4 | 12 | 0.28 |
| | | | | 5bvq | 607.2 | 3 | 0.16 |
| | | | | 5c00 | 915.8 | 149 | 0.83 |
| | | | | 5c86 | 431.7 | 0 | 0.12 |
| Average | 1635.0 | 111.7 | 0.68 | Average | 793.6 | 26.8 | 0.28 |
| Std Dev | 1029.7 | 98.7 | 0.27 | Std Dev | 528.2 | 62.5 | 0.26 |

[a] Test set selection was based on the following criteria: (1) PDB release date between January 2014 and August 2015; (2) no ligands in structure; (3) only a single type of protein in the structure, i.e., no heterodimers; and (4) the PDB file describes author determined biological units to assess the biological assembly as suggested by the authors.

**Table S10.** Classification of test set dimers by three methods[a,b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 3w66 | 0.12 | xtal | dimer | uncertain |
| 3w8g | 0.87 | xtal | dimer | stable |
| 3we1 | 0.13 | xtal | monomer | stable |
| 3wfi | 1.00 | bio | dimer | stable |
| 3wjk | 0.89 | bio | dimer | stable |
| 3wkw | 0.77 | bio | dimer | stable |
| 3wmd | 0.61 | bio | dimer | stable |
| 3wo8 | 0.81 | bio | dimer | stable |
| 3wpx | 0.86 | bio | dimer | uncertain |
| 3wsc | 0.13 | bio | dimer | stable |
| 3wtz | 0.74 | xtal | dimer | stable |
| 3wu0 | 0.78 | xtal | dimer | stable |
| 3wva | 0.83 | bio | dimer | stable |
| 3wvb | 0.84 | bio | dimer | stable |
| 3wvo | 0.76 | bio | dimer | stable |
| 3wvz | 0.77 | bio | tetramer | stable |
| 3wx4 | 0.84 | xtal | dimer | stable |
| 3wxi | 0.83 | bio | dimer | stable |
| 3wy7 | 0.82 | bio | dimer | stable |
| 3wyb | 0.80 | bio | dimer | stable |
| 3wyd | 0.72 | xtal | dimer | stable |
| 3wzg | 0.84 | bio | dimer | stable |
| 4bhy | 0.54 | bio | tetramer | stable |
| 4c7v | 0.76 | bio | dimer | stable |
| 4c88 | 0.79 | bio | 16-mer | stable |
| 4cbv | 0.65 | bio | dimer | stable |
| 4chk | 0.62 | bio | monomer | stable |
| 4cij | 0.54 | bio | dimer | stable |
| 4ckk | 0.66 | bio | dimer | stable |
| 4ckn | 0.77 | xtal | dimer | stable |
| 4cmz | 1.00 | bio | dimer | stable |
| 4cop | 0.83 | xtal | dimer | uncertain |
| 4cti | 0.70 | bio | dimer | stable |
| 4cu5 | 1.00 | bio | dimer | stable |
| 4cw9 | 0.12 | xtal | dimer | stable |
| 4cwc | 0.64 | bio | tetramer | stable |
| 4cwe | 0.48 | bio | dimer | stable |
| 4cxj | 0.83 | bio | dimer | stable |
| 4d28 | 0.51 | xtal | dimer | stable |
| 4d5s | 0.83 | bio | dimer | stable |
| 4d6k | 1.00 | bio | dimer | stable |
| 4fb8 | 0.81 | bio | dimer | stable |
| 4ihe | 0.82 | bio | tetramer | stable |
| 4j0e | 0.96 | bio | dimer | stable |
| 4j0f | 0.97 | bio | dimer | stable |
| 4j7a | 0.82 | bio | tetramer | stable |
| 4j7r | 1.00 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4jgm | 0.12 | bio | dimer | uncertain |
| 4jp2 | 0.47 | bio | tetramer | stable |
| 4ju5 | 0.97 | bio | dimer | stable |
| 4jup | 0.38 | xtal | dimer | uncertain |
| 4k2e | 0.84 | bio | dimer | stable |
| 4kde | 1.00 | bio | dimer | stable |
| 4ke2 | 0.18 | xtal | hexamer | stable |
| 4km3 | 0.83 | xtal | dimer | stable |
| 4kn8 | 1.00 | bio | dimer | stable |
| 4kp2 | 0.57 | bio | dimer | stable |
| 4kz1 | 0.81 | bio | dimer | stable |
| 4l2w | 0.61 | xtal | tetramer | stable |
| 4l4q | 0.74 | bio | tetramer | stable |
| 4l69 | 0.83 | bio | dimer | stable |
| 4l9e | 1.00 | bio | dimer | stable |
| 4le5 | 0.60 | bio | dimer | stable |
| 4lft | 0.12 | bio | monomer | stable |
| 4ljk | 0.89 | bio | dimer | uncertain |
| 4ljl | 0.96 | bio | dimer | stable |
| 4lpu | 0.80 | bio | tetramer | stable |
| 4lpw | 0.74 | bio | hexamer | stable |
| 4lpx | 0.63 | bio | hexamer | stable |
| 4ltb | 0.35 | bio | dimer | stable |
| 4luy | 0.82 | bio | dimer | stable |
| 4lwo | 0.81 | bio | dimer | stable |
| 4m0d | 0.66 | bio | tetramer | stable |
| 4m0q | 0.77 | xtal | dimer | stable |
| 4m23 | 0.78 | bio | dimer | stable |
| 4m36 | 0.61 | bio | dimer | stable |
| 4m6a | 0.82 | bio | dimer | stable |
| 4m8z | 0.81 | bio | dimer | stable |
| 4mac | 0.81 | bio | monomer | stable |
| 4mdu | 0.19 | xtal | dimer | stable |
| 4mea | 1.00 | bio | dimer | stable |
| 4mei | 0.31 | bio | dimer | stable |
| 4mfu | 0.12 | xtal | monomer | stable |
| 4mfv | 0.12 | xtal | monomer | stable |
| 4mid | 0.89 | bio | dimer | stable |
| 4mir | 0.87 | bio | dimer | stable |
| 4mis | 0.93 | bio | dimer | stable |
| 4ml3 | 0.64 | bio | dimer | uncertain |
| 4mld | 0.67 | bio | dodecamer | stable |
| 4mmn | 1.00 | bio | dimer | stable |
| 4mpl | 0.83 | bio | dimer | stable |
| 4mt8 | 0.61 | bio | tetramer | stable |
| 4mtx | 0.59 | bio | octomer | stable |
| 4muo | 0.81 | bio | dimer | stable |
| 4mxm | 0.83 | bio | dimer | stable |
| 4myc | 0.26 | bio | dimer | stable |
| 4myz | 1.00 | bio | dimer | stable |
| 4mzm | 1.00 | bio | dimer | stable |
| 4mzp | 0.99 | bio | dimer | stable |
| 4mzt | 0.86 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4n06 | 0.66 | bio | dimer | stable |
| 4n1k | 0.40 | bio | tetramer | stable |
| 4n1y | 0.87 | bio | dimer | stable |
| 4n92 | 0.12 | xtal | monomer | stable |
| 4n9h | 0.84 | bio | dimer | stable |
| 4na2 | 0.76 | bio | dimer | stable |
| 4ncd | 0.83 | xtal | monomer | stable |
| 4ndj | 0.73 | bio | tetramer | stable |
| 4ndk | 0.83 | bio | dimer | stable |
| 4ndw | 0.91 | bio | dimer | stable |
| 4nj0 | 1.00 | xtal | dimer | stable |
| 4nj1 | 0.98 | xtal | dimer | stable |
| 4nk7 | 0.60 | bio | tetramer | uncertain |
| 4nkk | 1.00 | bio | dimer | stable |
| 4nn1 | 1.00 | bio | dimer | stable |
| 4nom | 0.12 | xtal | dimer | uncertain |
| 4npu | 1.00 | bio | dimer | stable |
| 4nqf | 0.49 | xtal | dimer | stable |
| 4nqt | 0.72 | bio | dimer | stable |
| 4nsr | 0.83 | xtal | dimer | stable |
| 4nsw | 0.31 | bio | dimer | stable |
| 4ny0 | 0.12 | xtal | dimer | stable |
| 4o0q | 1.00 | bio | dimer | stable |
| 4o1h | 1.00 | bio | dimer | stable |
| 4o2h | 0.38 | xtal | dimer | stable |
| 4o60 | 0.13 | bio | dimer | stable |
| 4o8b | 1.00 | bio | dimer | stable |
| 4oaf | 0.46 | bio | monomer | stable |
| 4oft | 1.00 | bio | dimer | stable |
| 4ogd | 0.73 | bio | dimer | stable |
| 4ogf | 0.83 | bio | dimer | stable |
| 4oh9 | 0.83 | bio | dimer | stable |
| 4oi3 | 1.00 | bio | dimer | stable |
| 4okc | 0.83 | bio | dimer | stable |
| 4oky | 0.44 | xtal | dimer | stable |
| 4om7 | 0.49 | bio | dimer | stable |
| 4omt | 0.28 | bio | monomer | stable |
| 4ooi | 0.99 | bio | dimer | stable |
| 4or8 | 0.81 | bio | dimer | stable |
| 4otm | 0.83 | bio | dimer | stable |
| 4oun | 0.85 | bio | dimer | stable |
| 4p08 | 0.55 | xtal | dimer | stable |
| 4p12 | 0.54 | bio | dimer | stable |
| 4p22 | 0.66 | bio | dimer | stable |
| 4p61 | 1.00 | bio | dimer | stable |
| 4p6k | 0.23 | bio | tetramer | stable |
| 4p6l | 0.13 | xtal | dimer | stable |
| 4p96 | 0.80 | bio | dimer | stable |
| 4p9f | 0.81 | bio | hexamer | stable |
| 4pd0 | 0.56 | bio | dimer | stable |
| 4pdp | 0.12 | xtal | monomer | stable |
| 4pgg | 0.82 | bio | dimer | stable |
| 4ph6 | 0.83 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4pmu | 0.82 | bio | dimer | stable |
| 4pn0 | 0.85 | bio | dimer | stable |
| 4pon | 1.00 | bio | dimer | stable |
| 4prs | 0.82 | bio | dimer | stable |
| 4pu7 | 1.00 | xtal | dimer | stable |
| 4pu8 | 1.00 | xtal | dimer | stable |
| 4puh | 1.00 | bio | dimer | uncertain |
| 4pus | 0.12 | xtal | dimer | uncertain |
| 4pvc | 0.80 | xtal | monomer | stable |
| 4pz9 | 0.32 | bio | dimer | uncertain |
| 4pzc | 0.91 | bio | hexamer | stable |
| 4q0c | 0.73 | bio | dimer | stable |
| 4q20 | 0.81 | bio | tetramer | stable |
| 4q25 | 0.65 | bio | dimer | stable |
| 4q2o | 1.00 | bio | dimer | stable |
| 4q2q | 1.00 | bio | dimer | stable |
| 4q75 | 0.80 | bio | dimer | stable |
| 4q76 | 0.80 | bio | dimer | stable |
| 4q97 | 0.44 | bio | dimer | stable |
| 4q9b | 0.83 | xtal | dimer | stable |
| 4qfb | 0.12 | xtal | monomer | stable |
| 4qhr | 0.83 | bio | dimer | stable |
| 4qjn | 0.84 | bio | dimer | stable |
| 4ql6 | 0.12 | bio | dimer | uncertain |
| 4qr0 | 1.00 | bio | dimer | stable |
| 4qr1 | 1.00 | bio | dimer | stable |
| 4qr2 | 1.00 | bio | dimer | stable |
| 4qva | 0.32 | bio | dimer | stable |
| 4qvg | 0.88 | bio | dimer | stable |
| 4qvj | 0.32 | bio | dimer | stable |
| 4qxz | 0.82 | bio | dimer | uncertain |
| 4qyx | 0.22 | xtal | monomer | stable |
| 4r0b | 0.80 | bio | dimer | stable |
| 4r1i | 0.28 | bio | dimer | stable |
| 4r1n | 1.00 | bio | hexamer | stable |
| 4r27 | 0.12 | bio | monomer | stable |
| 4r3q | 0.79 | bio | hexamer | stable |
| 4r8e | 0.79 | bio | dimer | stable |
| 4ra8 | 0.15 | xtal | dimer | stable |
| 4rct | 0.80 | bio | dimer | stable |
| 4rd9 | 0.75 | bio | dimer | stable |
| 4rdj | 0.79 | xtal | dimer | stable |
| 4rg7 | 0.91 | bio | dimer | stable |
| 4rie | 0.75 | bio | dimer | stable |
| 4rmb | 0.95 | bio | dimer | stable |
| 4rni | 0.47 | bio | dimer | stable |
| 4rnj | 0.31 | xtal | monomer | stable |
| 4rns | 0.88 | bio | dimer | stable |
| 4rsj | 0.50 | bio | dimer | stable |
| 4rsw | 0.51 | bio | dimer | stable |
| 4rvs | 0.62 | bio | dimer | stable |
| 4ry2 | 0.38 | bio | dimer | stable |
| 4ryj | 0.12 | xtal | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4ryp | 0.82 | bio | dimer | stable |
| 4s03 | 0.62 | xtal | dimer | uncertain |
| 4s0j | 0.63 | xtal | dimer | uncertain |
| 4to7 | 1.00 | xtal | monomer | stable |
| 4tq7 | 0.81 | xtal | dimer | uncertain |
| 4tqj | 1.00 | xtal | monomer | stable |
| 4tr7 | 0.46 | bio | dimer | stable |
| 4trh | 0.33 | bio | dimer | stable |
| 4trt | 0.44 | bio | dimer | stable |
| 4ttw | 0.12 | xtal | dimer | stable |
| 4ttx | 1.00 | bio | dimer | stable |
| 4u2i | 1.00 | bio | dimer | uncertain |
| 4u2u | 0.71 | bio | dimer | stable |
| 4u3q | 0.12 | xtal | dimer | uncertain |
| 4u4i | 0.27 | bio | monomer | stable |
| 4u5h | 0.27 | xtal | dimer | stable |
| 4u64 | 0.83 | xtal | dimer | stable |
| 4u9c | 0.12 | xtal | monomer | stable |
| 4ua2 | 0.75 | bio | octomer | stable |
| 4uds | 0.87 | bio | dimer | stable |
| 4up8 | 0.77 | bio | dimer | stable |
| 4uu3 | 0.86 | bio | dimer | stable |
| 4uvj | 0.29 | xtal | dimer | stable |
| 4uzn | 0.12 | xtal | monomer | stable |
| 4v1p | 0.87 | xtal | dimer | stable |
| 4v2f | 0.82 | bio | dimer | stable |
| 4w4r | 0.51 | bio | dimer | stable |
| 4w69 | 0.67 | xtal | monomer | stable |
| 4w6a | 0.83 | xtal | monomer | stable |
| 4w6c | 0.76 | bio | dimer | stable |
| 4w6g | 0.83 | bio | monomer | stable |
| 4w6h | 0.73 | xtal | monomer | stable |
| 4w6i | 0.82 | xtal | monomer | stable |
| 4w6k | 0.76 | xtal | dimer | uncertain |
| 4w6l | 0.35 | xtal | tetramer | stable |
| 4w6n | 0.72 | xtal | monomer | stable |
| 4w6o | 0.82 | xtal | tetramer | stable |
| 4w6p | 0.67 | xtal | monomer | stable |
| 4w6r | 0.79 | xtal | monomer | stable |
| 4w7x | 0.77 | xtal | monomer | stable |
| 4w8i | 0.78 | bio | dimer | stable |
| 4wd9 | 0.61 | bio | dimer | stable |
| 4whj | 0.66 | bio | dimer | stable |
| 4wic | 0.34 | bio | dimer | stable |
| 4wij | 0.44 | bio | dimer | stable |
| 4wik | 0.46 | bio | dimer | stable |
| 4wja | 1.00 | bio | dimer | stable |
| 4wnz | 0.65 | bio | monomer | stable |
| 4wo7 | 1.00 | bio | dimer | stable |
| 4wpe | 0.64 | bio | dimer | stable |
| 4wse | 0.60 | bio | dimer | stable |
| 4wt5 | 0.81 | bio | dimer | stable |
| 4wum | 0.78 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4wy8 | 0.75 | bio | dimer | stable |
| 4x0r | 0.85 | bio | dimer | stable |
| 4x5n | 0.58 | bio | dimer | stable |
| 4x5u | 0.51 | bio | dimer | stable |
| 4x8f | 1.00 | bio | dimer | stable |
| 4xa1 | 0.27 | bio | dimer | stable |
| 4xa3 | 0.29 | bio | dimer | stable |
| 4xa4 | 0.42 | bio | dimer | stable |
| 4xa6 | 0.24 | bio | octomer | stable |
| 4xbx | 0.92 | bio | dimer | stable |
| 4xlx | 0.75 | bio | dimer | stable |
| 4xo1 | 0.94 | bio | dimer | stable |
| 4xo2 | 1.00 | bio | dimer | stable |
| 4xoh | 0.20 | bio | dimer | stable |
| 4xws | 0.62 | bio | dimer | stable |
| 4xyg | 0.88 | bio | dimer | stable |
| 4xz7 | 0.79 | bio | dimer | stable |
| 4y0m | 0.79 | bio | dimer | stable |
| 4y9a | 0.99 | bio | dimer | stable |
| 4ylt | 0.87 | bio | dimer | stable |
| 4ymr | 0.76 | bio | dimer | stable |
| 4ynh | 1.00 | bio | dimer | stable |
| 4yub | 0.74 | bio | dimer | stable |
| 4yzy | 0.55 | bio | dimer | stable |
| 4z27 | 0.80 | bio | dimer | stable |
| 4z6j | 0.84 | bio | octomer | stable |
| 4zbh | 0.85 | bio | dimer | uncertain |
| 4zbw | 0.12 | xtal | monomer | stable |
| 4zm8 | 0.58 | bio | dimer | stable |
| 4zqa | 0.68 | xtal | dimer | stable |
| 5a0o | 0.12 | bio | dimer | stable |
| 5a2n | 0.12 | xtal | dimer | stable |
| 5a48 | 0.13 | bio | dimer | uncertain |
| 5bto | 0.40 | bio | monomer | stable |

[a] yellow: incorrect classification
[b] Criteria for test selection are given in Table S9

**Table S11.** Classification of test set monomers by three methods[a,b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 3w6r | 0.65 | xtal | monomer | stable |
| 3w94 | 0.12 | xtal | monomer | stable |
| 3w9g | 0.23 | xtal | dimer | stable |
| 3wbi | 0.12 | bio | monomer | stable |
| 3wbj | 0.68 | xtal | monomer | stable |
| 3wdf | 0.58 | xtal | monomer | stable |
| 3wea | 0.12 | xtal | dimer | stable |
| 3who | 0.13 | bio | monomer | stable |
| 3wj9 | 0.12 | xtal | monomer | stable |
| 3wo9 | 0.12 | bio | monomer | stable |
| 3wob | 0.13 | xtal | monomer | stable |
| 3wp3 | 0.12 | xtal | monomer | stable |
| 3wp9 | 0.41 | xtal | dimer | stable |
| 3wpj | 0.12 | bio | monomer | stable |
| 3wpy | 0.19 | xtal | monomer | stable |
| 3wpz | 0.43 | xtal | monomer | stable |
| 3wrt | 0.12 | xtal | monomer | stable |
| 3wuq | 0.12 | xtal | monomer | stable |
| 3wuy | 0.12 | bio | dimer | stable |
| 3wv4 | 0.12 | xtal | monomer | stable |
| 3wvf | 0.12 | xtal | monomer | stable |
| 3wvt | 0.12 | xtal | monomer | stable |
| 3wx5 | 0.12 | xtal | monomer | stable |
| 3wzt | 0.29 | xtal | monomer | stable |
| 3x0w | 0.12 | bio | monomer | stable |
| 3zfm | 0.12 | xtal | monomer | stable |
| 3zfy | 0.12 | xtal | monomer | stable |
| 3zk0 | 0.22 | xtal | monomer | stable |
| 3zlh | 0.80 | bio | octomer | stable |
| 3zm0 | 0.12 | xtal | monomer | stable |
| 3zm1 | 0.12 | xtal | monomer | stable |
| 3zm2 | 0.12 | xtal | monomer | stable |
| 3zm3 | 0.12 | xtal | monomer | stable |
| 3zny | 0.12 | xtal | monomer | stable |
| 3zq3 | 0.26 | xtal | monomer | stable |
| 4bg0 | 0.12 | xtal | monomer | stable |
| 4bob | 0.12 | xtal | monomer | stable |
| 4bod | 0.12 | xtal | monomer | stable |
| 4bp8 | 0.64 | bio | dimer | stable |
| 4bpf | 0.15 | xtal | monomer | stable |
| 4bpy | 0.12 | xtal | monomer | stable |
| 4bxm | 0.12 | xtal | monomer | stable |
| 4c41 | 0.12 | bio | monomer | stable |
| 4c5f | 0.12 | xtal | monomer | stable |
| 4c6r | 0.27 | xtal | monomer | stable |
| 4cbe | 0.12 | xtal | monomer | stable |
| 4cbh | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4cbi | 0.12 | xtal | monomer | stable |
| 4cbl | 0.20 | bio | dimer | stable |
| 4cbm | 0.12 | bio | dimer | uncertain |
| 4cdo | 0.38 | xtal | monomer | stable |
| 4cfi | 0.12 | bio | monomer | stable |
| 4ch7 | 0.12 | xtal | monomer | stable |
| 4chj | 0.83 | xtal | tetramer | uncertain |
| 4cil | 0.15 | xtal | monomer | stable |
| 4co7 | 0.12 | xtal | monomer | stable |
| 4cso | 0.19 | xtal | monomer | stable |
| 4cx8 | 0.12 | bio | dimer | stable |
| 4cxi | 0.83 | bio | dimer | stable |
| 4cye | 0.83 | bio | dimer | stable |
| 4d2o | 0.12 | xtal | monomer | stable |
| 4d4q | 0.12 | xtal | monomer | stable |
| 4d5r | 0.81 | bio | dimer | stable |
| 4d70 | 0.12 | xtal | monomer | stable |
| 4d7r | 0.12 | xtal | monomer | stable |
| 4h9w | 0.15 | xtal | monomer | stable |
| 4hic | 0.12 | xtal | monomer | stable |
| 4icu | 0.12 | xtal | monomer | stable |
| 4ino | 0.12 | xtal | monomer | stable |
| 4iqc | 0.13 | xtal | monomer | stable |
| 4irf | 0.40 | xtal | monomer | stable |
| 4it7 | 0.12 | xtal | monomer | stable |
| 4iyc | 0.12 | xtal | monomer | stable |
| 4ize | 0.29 | xtal | monomer | stable |
| 4izl | 0.12 | xtal | monomer | stable |
| 4j0o | 0.12 | xtal | monomer | stable |
| 4j1s | 0.16 | xtal | monomer | stable |
| 4j2r | 0.12 | xtal | monomer | stable |
| 4jkq | 0.12 | bio | monomer | stable |
| 4jmp | 0.12 | xtal | monomer | stable |
| 4k1s | 0.12 | xtal | monomer | stable |
| 4k40 | 0.12 | xtal | monomer | stable |
| 4k51 | 0.12 | xtal | trimer | stable |
| 4k5q | 0.12 | xtal | monomer | stable |
| 4k82 | 0.12 | xtal | monomer | stable |
| 4k83 | 0.55 | xtal | monomer | stable |
| 4k9s | 0.12 | xtal | monomer | stable |
| 4kex | 0.12 | xtal | monomer | stable |
| 4kxo | 0.87 | bio | dimer | stable |
| 4l1d | 0.43 | xtal | monomer | stable |
| 4l6u | 0.12 | xtal | monomer | stable |
| 4l8i | 0.12 | xtal | dimer | stable |
| 4l8l | 0.83 | bio | dimer | uncertain |
| 4l9h | 0.78 | bio | monomer | stable |
| 4lcm | 0.12 | xtal | dimer | stable |
| 4lee | 0.12 | xtal | monomer | stable |
| 4lhf | 0.83 | bio | monomer | stable |
| 4lk4 | 0.24 | bio | monomer | stable |
| 4lpt | 0.56 | bio | hexamer | stable |
| 4lrk | 0.83 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4lso | 0.12 | bio | monomer | stable |
| 4ltt | 0.12 | xtal | monomer | stable |
| 4lw5 | 0.13 | xtal | monomer | stable |
| 4lzi | 0.70 | xtal | monomer | stable |
| 4m64 | 0.12 | xtal | monomer | stable |
| 4m7g | 0.12 | bio | monomer | stable |
| 4m80 | 0.12 | xtal | monomer | stable |
| 4m8g | 0.38 | xtal | monomer | stable |
| 4m90 | 0.12 | xtal | monomer | stable |
| 4m9p | 0.34 | xtal | monomer | stable |
| 4mc0 | 0.12 | xtal | monomer | stable |
| 4mck | 0.44 | xtal | monomer | stable |
| 4mee | 0.12 | xtal | monomer | stable |
| 4mel | 0.87 | bio | dimer | stable |
| 4mem | 0.42 | bio | dimer | stable |
| 4mfi | 0.38 | bio | monomer | stable |
| 4mfj | 0.13 | xtal | monomer | stable |
| 4mgf | 0.45 | xtal | monomer | stable |
| 4mgs | 0.12 | xtal | monomer | stable |
| 4mhp | 0.12 | xtal | monomer | stable |
| 4mhr | 1.00 | bio | dimer | stable |
| 4mq3 | 0.12 | bio | monomer | stable |
| 4mt5 | 0.24 | xtal | monomer | stable |
| 4mt6 | 0.12 | xtal | monomer | stable |
| 4mt7 | 0.12 | xtal | monomer | stable |
| 4mzd | 0.12 | xtal | monomer | stable |
| 4n08 | 0.12 | xtal | monomer | stable |
| 4n1l | 0.24 | xtal | monomer | stable |
| 4n3x | 0.82 | xtal | tetramer | stable |
| 4n40 | 0.12 | xtal | trimer | stable |
| 4n4a | 0.19 | bio | dimer | stable |
| 4n5a | 0.12 | xtal | monomer | stable |
| 4n5c | 0.12 | xtal | monomer | stable |
| 4n5q | 0.15 | xtal | monomer | stable |
| 4n6l | 0.20 | xtal | monomer | stable |
| 4n6t | 0.12 | xtal | monomer | stable |
| 4n6u | 0.12 | xtal | monomer | stable |
| 4n75 | 0.12 | xtal | monomer | stable |
| 4n7f | 0.83 | xtal | dimer | stable |
| 4n8h | 0.53 | bio | monomer | stable |
| 4n8k | 0.58 | bio | monomer | stable |
| 4n8l | 0.48 | bio | monomer | stable |
| 4nbo | 0.53 | xtal | monomer | stable |
| 4nc9 | 0.43 | bio | dimer | stable |
| 4nci | 0.65 | xtal | monomer | stable |
| 4ndl | 0.12 | xtal | monomer | stable |
| 4nfb | 0.12 | xtal | monomer | stable |
| 4nfc | 0.50 | xtal | monomer | stable |
| 4nfx | 1.00 | bio | dimer | stable |
| 4ng0 | 1.00 | xtal | monomer | stable |
| 4nj6 | 0.67 | bio | dimer | uncertain |
| 4nj7 | 0.12 | xtal | monomer | stable |
| 4nj8 | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4njc | 1.00 | xtal | monomer | stable |
| 4nk6 | 0.34 | bio | dimer | stable |
| 4nk8 | 0.77 | bio | dimer | stable |
| 4nl7 | 0.12 | xtal | dimer | stable |
| 4nlb | 0.12 | xtal | monomer | stable |
| 4nng | 0.12 | xtal | monomer | stable |
| 4nnh | 0.27 | xtal | monomer | stable |
| 4nnk | 0.12 | xtal | monomer | stable |
| 4noj | 0.12 | xtal | monomer | stable |
| 4npf | 0.86 | bio | dimer | uncertain |
| 4nq0 | 0.12 | xtal | monomer | stable |
| 4nsp | 0.12 | xtal | monomer | stable |
| 4nu2 | 0.12 | xtal | monomer | stable |
| 4nv8 | 0.74 | xtal | dimer | stable |
| 4nx9 | 0.68 | bio | monomer | stable |
| 4nzz | 0.12 | xtal | monomer | stable |
| 4o2x | 0.32 | xtal | monomer | stable |
| 4o3x | 0.12 | xtal | monomer | stable |
| 4o4c | 0.41 | xtal | monomer | stable |
| 4o5p | 0.12 | xtal | monomer | stable |
| 4o5s | 0.12 | xtal | monomer | stable |
| 4o6g | 0.13 | xtal | monomer | stable |
| 4o6k | 0.20 | xtal | monomer | stable |
| 4o6x | 0.83 | xtal | dimer | uncertain |
| 4o7q | 0.12 | xtal | monomer | stable |
| 4o8s | 0.13 | xtal | monomer | stable |
| 4o8v | 0.12 | xtal | monomer | stable |
| 4o9f | 0.12 | xtal | monomer | stable |
| 4o9l | 0.19 | xtal | monomer | stable |
| 4oa6 | 0.12 | xtal | monomer | stable |
| 4ob4 | 0.70 | bio | dimer | stable |
| 4od4 | 0.12 | xtal | dimer | stable |
| 4od6 | 0.12 | xtal | monomer | stable |
| 4odd | 0.76 | xtal | monomer | stable |
| 4of0 | 0.12 | xtal | monomer | stable |
| 4of5 | 0.12 | bio | monomer | stable |
| 4ofv | 0.12 | bio | monomer | stable |
| 4ohd | 0.12 | xtal | monomer | stable |
| 4ohe | 0.12 | xtal | monomer | stable |
| 4ohh | 0.12 | xtal | monomer | stable |
| 4ohi | 0.12 | xtal | monomer | stable |
| 4ohl | 0.12 | xtal | monomer | stable |
| 4ohr | 1.00 | bio | dimer | stable |
| 4oj0 | 0.83 | xtal | dimer | stable |
| 4ok0 | 0.12 | xtal | monomer | stable |
| 4om9 | 0.12 | xtal | monomer | stable |
| 4oq1 | 0.12 | xtal | monomer | stable |
| 4oqw | 1.00 | bio | dimer | stable |
| 4orw | 0.12 | xtal | monomer | stable |
| 4os0 | 1.00 | xtal | dimer | stable |
| 4os3 | 1.00 | xtal | dimer | stable |
| 4os8 | 1.00 | xtal | dimer | stable |
| 4otd | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4ou0 | 0.22 | xtal | monomer | stable |
| 4ow6 | 0.12 | xtal | monomer | stable |
| 4oyl | 0.12 | xtal | trimer | uncertain |
| 4oyy | 0.12 | xtal | trimer | stable |
| 4ozk | 0.12 | xtal | monomer | stable |
| 4p09 | 0.12 | xtal | monomer | stable |
| 4p0f | 0.36 | xtal | dimer | stable |
| 4p0j | 0.63 | xtal | monomer | stable |
| 4p0k | 0.79 | xtal | monomer | stable |
| 4p0l | 0.20 | xtal | monomer | stable |
| 4p0m | 0.19 | xtal | hexamer | stable |
| 4p0o | 0.41 | xtal | monomer | stable |
| 4p0y | 0.12 | xtal | monomer | stable |
| 4p0z | 0.12 | xtal | monomer | stable |
| 4p17 | 0.13 | xtal | monomer | stable |
| 4p39 | 0.40 | bio | tetramer | stable |
| 4p47 | 0.12 | xtal | monomer | stable |
| 4p48 | 0.12 | xtal | monomer | stable |
| 4p5u | 0.12 | xtal | monomer | stable |
| 4p7o | 0.16 | xtal | dimer | stable |
| 4pa1 | 0.67 | xtal | dimer | stable |
| 4pbd | 0.58 | xtal | monomer | stable |
| 4pcf | 0.12 | bio | trimer | uncertain |
| 4pd3 | 0.23 | bio | monomer | stable |
| 4pej | 0.60 | bio | dimer | stable |
| 4pek | 0.12 | bio | monomer | stable |
| 4pgr | 0.12 | xtal | monomer | stable |
| 4pgs | 0.12 | xtal | dimer | stable |
| 4pgu | 0.15 | xtal | monomer | stable |
| 4pgv | 0.13 | xtal | monomer | stable |
| 4ph1 | 0.73 | xtal | trimer | stable |
| 4pjq | 0.20 | bio | dimer | stable |
| 4pk1 | 0.12 | xtal | monomer | stable |
| 4pk9 | 0.78 | bio | dimer | stable |
| 4pka | 0.81 | bio | dimer | stable |
| 4pkx | 0.12 | xtal | monomer | stable |
| 4pmh | 0.12 | xtal | monomer | stable |
| 4pn7 | 0.12 | bio | monomer | stable |
| 4po4 | 0.12 | xtal | monomer | stable |
| 4poy | 0.12 | xtal | monomer | stable |
| 4ppj | 0.12 | bio | monomer | stable |
| 4ppk | 0.12 | bio | monomer | stable |
| 4ppl | 0.12 | xtal | monomer | stable |
| 4pqo | 0.12 | xtal | monomer | stable |
| 4pqz | 0.12 | xtal | dimer | uncertain |
| 4psd | 0.12 | xtal | monomer | stable |
| 4psf | 0.23 | bio | monomer | stable |
| 4pug | 0.12 | bio | dimer | stable |
| 4pui | 0.12 | xtal | monomer | stable |
| 4pwq | 0.13 | xtal | dimer | uncertain |
| 4pzp | 0.12 | xtal | monomer | stable |
| 4q2s | 0.12 | xtal | monomer | stable |
| 4q2y | 0.23 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4q3h | 0.85 | xtal | monomer | stable |
| 4q4g | 0.12 | xtal | monomer | stable |
| 4q4n | 0.12 | xtal | monomer | stable |
| 4q5y | 0.23 | xtal | dimer | stable |
| 4q65 | 0.12 | xtal | monomer | stable |
| 4q6l | 0.12 | xtal | monomer | stable |
| 4q6v | 0.12 | xtal | monomer | stable |
| 4q6z | 0.12 | xtal | dimer | uncertain |
| 4q7k | 0.12 | xtal | monomer | stable |
| 4q7m | 0.84 | bio | dimer | stable |
| 4q7t | 0.12 | xtal | monomer | stable |
| 4q9h | 0.12 | xtal | monomer | stable |
| 4q9p | 0.68 | xtal | tetramer | uncertain |
| 4qaj | 0.60 | xtal | monomer | stable |
| 4qaz | 0.13 | xtal | monomer | stable |
| 4qb0 | 0.12 | xtal | monomer | stable |
| 4qbe | 0.43 | xtal | monomer | stable |
| 4qcj | 0.31 | bio | monomer | stable |
| 4qdr | 0.12 | xtal | monomer | stable |
| 4qdt | 0.12 | xtal | monomer | stable |
| 4qdu | 0.12 | xtal | monomer | stable |
| 4qgy | 0.12 | bio | monomer | stable |
| 4qlo | 0.80 | bio | dimer | stable |
| 4qlr | 0.15 | xtal | monomer | stable |
| 4qmd | 0.12 | xtal | monomer | stable |
| 4qmi | 0.12 | xtal | monomer | stable |
| 4qmj | 0.12 | xtal | monomer | stable |
| 4qs8 | 0.12 | xtal | monomer | stable |
| 4qt4 | 0.12 | xtal | monomer | stable |
| 4qtz | 0.12 | xtal | monomer | stable |
| 4quc | 0.12 | xtal | monomer | stable |
| 4quk | 0.12 | xtal | monomer | stable |
| 4qx0 | 0.28 | xtal | monomer | stable |
| 4qx1 | 0.20 | xtal | monomer | stable |
| 4qx2 | 0.27 | xtal | monomer | stable |
| 4qx3 | 0.24 | xtal | monomer | stable |
| 4qxl | 0.12 | xtal | monomer | stable |
| 4r05 | 0.12 | xtal | monomer | stable |
| 4r0e | 0.48 | xtal | monomer | stable |
| 4r0x | 0.12 | xtal | dimer | stable |
| 4r0y | 0.12 | xtal | monomer | stable |
| 4r19 | 0.12 | xtal | monomer | stable |
| 4r1a | 0.12 | xtal | monomer | stable |
| 4r1b | 0.12 | xtal | monomer | stable |
| 4r1c | 0.12 | xtal | monomer | stable |
| 4r58 | 0.12 | xtal | monomer | stable |
| 4r61 | 0.49 | xtal | monomer | stable |
| 4r6f | 0.12 | xtal | monomer | stable |
| 4r7v | 0.18 | bio | dimer | stable |
| 4r8r | 0.12 | xtal | monomer | stable |
| 4rcw | 0.40 | bio | dimer | uncertain |
| 4rdp | 0.82 | bio | monomer | stable |
| 4reh | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4rej | 0.12 | xtal | monomer | stable |
| 4rf6 | 0.12 | xtal | monomer | stable |
| 4rid | 0.18 | bio | tetramer | stable |
| 4rl1 | 0.12 | xtal | monomer | stable |
| 4rl9 | 0.12 | xtal | tetramer | stable |
| 4rlb | 0.12 | bio | tetramer | stable |
| 4rlm | 0.12 | xtal | monomer | stable |
| 4rln | 0.12 | bio | monomer | stable |
| 4ro1 | 0.12 | xtal | monomer | stable |
| 4roa | 0.45 | xtal | monomer | stable |
| 4rs6 | 0.82 | bio | hexamer | stable |
| 4rsq | 0.46 | xtal | monomer | stable |
| 4rsx | 0.12 | xtal | monomer | stable |
| 4rtd | 0.13 | xtal | monomer | stable |
| 4rth | 0.49 | xtal | monomer | stable |
| 4rwi | 0.66 | xtal | dimer | stable |
| 4rwq | 0.12 | xtal | monomer | stable |
| 4rwr | 0.78 | xtal | monomer | stable |
| 4rwu | 0.60 | xtal | monomer | stable |
| 4rwz | 0.79 | xtal | monomer | stable |
| 4ry4 | 0.12 | xtal | monomer | stable |
| 4ry6 | 0.12 | xtal | monomer | stable |
| 4ry7 | 0.12 | xtal | monomer | stable |
| 4rz2 | 0.12 | xtal | monomer | stable |
| 4s11 | 0.12 | xtal | monomer | stable |
| 4s3l | 0.15 | xtal | monomer | stable |
| 4s3p | 0.60 | xtal | tetramer | stable |
| 4tks | 0.58 | bio | monomer | stable |
| 4tlp | 0.12 | xtal | monomer | stable |
| 4tlw | 0.12 | xtal | monomer | stable |
| 4tn9 | 0.12 | xtal | monomer | stable |
| 4tnm | 0.12 | xtal | monomer | stable |
| 4tql | 0.12 | xtal | monomer | stable |
| 4tr5 | 1.00 | bio | monomer | stable |
| 4trk | 0.12 | xtal | monomer | stable |
| 4tse | 0.44 | xtal | dimer | stable |
| 4ttl | 0.12 | xtal | nopred | n/a |
| 4ttp | 0.12 | xtal | monomer | stable |
| 4tum | 0.27 | xtal | monomer | stable |
| 4tut | 0.80 | xtal | monomer | stable |
| 4tuu | 0.12 | xtal | monomer | stable |
| 4tve | 0.15 | xtal | monomer | stable |
| 4tx2 | 0.12 | xtal | monomer | stable |
| 4txp | 0.12 | xtal | monomer | stable |
| 4tza | 0.24 | xtal | monomer | stable |
| 4tzg | 0.80 | xtal | monomer | stable |
| 4tzi | 0.12 | xtal | monomer | stable |
| 4tzj | 0.12 | xtal | monomer | stable |
| 4u0l | 0.12 | xtal | monomer | stable |
| 4u1d | 0.16 | xtal | monomer | stable |
| 4u2m | 0.34 | xtal | tetramer | stable |
| 4u2n | 1.00 | xtal | dimer | stable |
| 4u3a | 0.92 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 4u3h | 0.12 | xtal | monomer | stable |
| 4u3t | 0.15 | xtal | monomer | stable |
| 4u3v | 0.12 | xtal | monomer | stable |
| 4u48 | 0.39 | bio | monomer | stable |
| 4u4h | 0.13 | bio | dimer | stable |
| 4u4j | 0.42 | bio | monomer | stable |
| 4u59 | 0.42 | bio | monomer | stable |
| 4u5a | 0.12 | xtal | monomer | stable |
| 4u9q | 0.46 | xtal | dimer | uncertain |
| 4ud5 | 0.12 | xtal | dimer | stable |
| 4uex | 0.12 | bio | monomer | stable |
| 4ulw | 0.83 | xtal | monomer | stable |
| 4umg | 0.24 | bio | dimer | uncertain |
| 4ums | 0.20 | xtal | monomer | stable |
| 4uos | 0.40 | xtal | monomer | stable |
| 4uts | 0.12 | xtal | monomer | stable |
| 4uu4 | 0.34 | bio | monomer | stable |
| 4uv2 | 0.76 | bio | 16-mer | stable |
| 4uv6 | 0.74 | xtal | monomer | stable |
| 4uvk | 0.12 | xtal | monomer | stable |
| 4uw2 | 0.12 | xtal | monomer | stable |
| 4uww | 1.00 | xtal | monomer | stable |
| 4uy3 | 0.12 | xtal | monomer | stable |
| 4uz2 | 0.19 | xtal | octomer | stable |
| 4v0t | 0.83 | bio | dimer | stable |
| 4v14 | 0.12 | xtal | monomer | stable |
| 4v16 | 0.12 | xtal | monomer | stable |
| 4v2b | 0.12 | xtal | monomer | stable |
| 4v2d | 0.12 | xtal | monomer | stable |
| 4v2e | 0.12 | bio | monomer | stable |
| 4v2u | 0.12 | xtal | monomer | stable |
| 4v38 | 0.12 | xtal | monomer | stable |
| 4v39 | 0.12 | xtal | monomer | stable |
| 4w4m | 0.12 | bio | monomer | stable |
| 4w5x | 0.35 | xtal | dimer | stable |
| 4w60 | 0.54 | xtal | dimer | stable |
| 4w6v | 0.12 | xtal | monomer | stable |
| 4w7g | 0.12 | xtal | monomer | stable |
| 4w8v | 1.00 | bio | tetramer | stable |
| 4w8w | 0.82 | bio | monomer | stable |
| 4w8z | 0.83 | bio | dimer | stable |
| 4wau | 0.33 | xtal | dimer | uncertain |
| 4wbz | 0.40 | xtal | monomer | stable |
| 4wdc | 0.12 | xtal | monomer | stable |
| 4we2 | 0.12 | xtal | monomer | stable |
| 4wfi | 0.12 | xtal | monomer | stable |
| 4wj1 | 0.50 | bio | dimer | stable |
| 4wj2 | 0.12 | bio | monomer | stable |
| 4wjs | 0.12 | xtal | monomer | stable |
| 4wmg | 0.12 | bio | monomer | stable |
| 4wo8 | 0.12 | xtal | monomer | stable |
| 4woy | 0.59 | bio | tetramer | stable |
| 4wp6 | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4wt3 | 0.12 | xtal | monomer | stable |
| 4wtx | 0.16 | xtal | monomer | stable |
| 4wu0 | 0.27 | xtal | monomer | stable |
| 4wz0 | 0.62 | xtal | dimer | stable |
| 4x0j | 0.12 | xtal | monomer | stable |
| 4x2m | 0.12 | xtal | monomer | stable |
| 4x2w | 0.59 | bio | tetramer | stable |
| 4x2x | 0.18 | bio | monomer | stable |
| 4x2y | 0.54 | xtal | monomer | stable |
| 4x3x | 0.12 | xtal | dimer | stable |
| 4x43 | 0.12 | bio | monomer | uncertain |
| 4x8h | 0.20 | bio | monomer | stable |
| 4x8m | 0.12 | xtal | monomer | stable |
| 4x9u | 0.12 | xtal | monomer | stable |
| 4xah | 1.00 | xtal | monomer | stable |
| 4xeh | 0.52 | bio | dimer | stable |
| 4xfu | 0.12 | xtal | dimer | stable |
| 4xfv | 0.12 | xtal | dimer | uncertain |
| 4xh3 | 0.12 | bio | dimer | uncertain |
| 4xhm | 0.16 | xtal | monomer | stable |
| 4xkk | 0.13 | xtal | monomer | stable |
| 4xm4 | 0.76 | bio | dimer | stable |
| 4xp8 | 0.34 | xtal | monomer | stable |
| 4xpk | 0.12 | xtal | monomer | stable |
| 4xq7 | 0.12 | xtal | monomer | stable |
| 4xy3 | 0.12 | xtal | monomer | stable |
| 4xzg | 0.12 | xtal | monomer | stable |
| 4y21 | 0.46 | bio | monomer | stable |
| 4y4q | 0.24 | xtal | dimer | stable |
| 4y5j | 0.33 | bio | dimer | stable |
| 4yeq | 0.34 | xtal | monomer | stable |
| 4yf2 | 0.12 | xtal | monomer | stable |
| 4yfe | 0.12 | xtal | monomer | stable |
| 4yfs | 0.12 | xtal | monomer | stable |
| 4yhe | 0.12 | xtal | monomer | stable |
| 4ykc | 0.40 | xtal | tetramer | stable |
| 4ykd | 0.12 | xtal | monomer | stable |
| 4yno | 0.12 | xtal | monomer | stable |
| 4ynv | 0.92 | xtal | monomer | stable |
| 4ynw | 1.00 | bio | dimer | stable |
| 4ypj | 0.12 | xtal | monomer | stable |
| 4yuo | 0.12 | xtal | monomer | stable |
| 4yvm | 0.38 | xtal | dimer | stable |
| 4yvo | 0.12 | xtal | monomer | stable |
| 4z29 | 0.47 | xtal | monomer | stable |
| 4z99 | 0.12 | xtal | monomer | stable |
| 4z9p | 0.72 | xtal | monomer | stable |
| 4zf3 | 0.32 | xtal | monomer | stable |
| 4zf4 | 0.40 | xtal | monomer | stable |
| 4zf5 | 0.54 | xtal | monomer | stable |
| 4zg1 | 0.12 | xtal | hexamer | uncertain |
| 4zj2 | 0.12 | xtal | monomer | stable |
| 4zj3 | 0.12 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4zmd | 0.12 | xtal | monomer | stable |
| 4zot | 0.12 | xtal | monomer | stable |
| 4zov | 0.84 | xtal | dimer | uncertain |
| 4zoy | 0.12 | xtal | monomer | stable |
| 4zuz | 0.19 | xtal | monomer | stable |
| 4zwj | 0.12 | xtal | monomer | stable |
| 5a0g | 0.12 | xtal | monomer | stable |
| 5a0z | 0.54 | bio | tetramer | stable |
| 5aem | 0.18 | xtal | monomer | stable |
| 5af5 | 0.12 | xtal | monomer | stable |
| 5aio | 0.81 | xtal | monomer | stable |
| 5aj8 | 0.12 | xtal | monomer | stable |
| 5avg | 0.29 | xtal | monomer | stable |
| 5avh | 0.79 | bio | tetramer | stable |
| 5brl | 0.19 | xtal | monomer | stable |
| 5bth | 0.28 | bio | monomer | stable |
| 5bvq | 0.16 | xtal | monomer | stable |
| 5c00 | 0.83 | bio | monomer | stable |
| 5c86 | 0.12 | xtal | monomer | stable |

[a] yellow: incorrect classification

[b] Criteria for test selection are given in Table S9

**Table S12.** Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the "difficult" subset of the test set[a]

| Biological dimers | | | | Crystallographic dimers | | | |
|---|---|---|---|---|---|---|---|
| PDB ID | Interface area (Å²) | $N_{nn}$ | Probability (dimer) | PDB ID | Interface area (Å²) | $N_{nn}$ | Probability (dimer) |
| 3w66 | 529.6 | 0 | 0.05 | 3w9g | 604.3 | 8 | 0.17 |
| 3w8g | 760.8 | 183 | 0.91 | 3wea | 445.6 | 0 | 0.05 |
| 3wtz | 690.6 | 74 | 0.75 | 3wp9 | 716.5 | 23 | 0.36 |
| 3wx4 | 1220.4 | 159 | 0.89 | 3wpj | 566.9 | 0 | 0.05 |
| 3wyd | 542.7 | 68 | 0.73 | 4c41 | 620.9 | 0 | 0.05 |
| 4chk | 743.5 | 49 | 0.61 | 4cbm | 1180.1 | 0 | 0.05 |
| 4ckn | 1371.7 | 82 | 0.79 | 4cfi | 628.2 | 0 | 0.05 |
| 4cop | 489.0 | 131 | 0.87 | 4chj | 930.5 | 144 | 0.88 |
| 4cw9 | 635.1 | 0 | 0.05 | 4d5r | 790.3 | 109 | 0.85 |
| 4cwc | 1505.3 | 52 | 0.63 | 4k51 | 874.1 | 0 | 0.05 |
| 4d28 | 1404.9 | 34 | 0.48 | 4l8i | 827.8 | 0 | 0.05 |
| 4jgm | 698.2 | 0 | 0.05 | 4l9h | 1109.1 | 85 | 0.80 |
| 4jup | 389.5 | 20 | 0.33 | 4lcm | 814.0 | 0 | 0.05 |
| 4ke2 | 1787.5 | 4 | 0.11 | 4lhf | 1034.8 | 148 | 0.88 |
| 4km3 | 1157.9 | 125 | 0.87 | 4lk4 | 595.0 | 9 | 0.18 |
| 4kp2 | 1756.8 | 41 | 0.54 | 4lso | 524.0 | 0 | 0.05 |
| 4l2w | 1072.2 | 47 | 0.59 | 4m7g | 499.9 | 0 | 0.05 |
| 4lft | 517.9 | 0 | 0.05 | 4mfi | 957.9 | 20 | 0.33 |
| 4m0q | 1449.4 | 83 | 0.79 | 4n3x | 940.2 | 122 | 0.87 |
| 4m23 | 1547.5 | 86 | 0.80 | 4n40 | 654.7 | 0 | 0.05 |
| 4mdu | 943.7 | 5 | 0.12 | 4n7f | 626.1 | 142 | 0.88 |
| 4nj0 | 882.7 | 229 | 1.00 | 4n8h | 1844.3 | 36 | 0.50 |
| 4nqf | 1203.6 | 32 | 0.46 | 4nl7 | 1254.8 | 0 | 0.05 |
| 4nsr | 1126.8 | 138 | 0.88 | 4npf | 1404.4 | 182 | 0.91 |
| 4ny0 | 735.5 | 0 | 0.05 | 4nv8 | 837.6 | 73 | 0.75 |
| 4o2h | 919.3 | 20 | 0.33 | 4nx9 | 1116.7 | 58 | 0.67 |
| 4oaf | 1130.5 | 28 | 0.42 | 4o6x | 616.0 | 151 | 0.88 |
| 4oky | 811.4 | 26 | 0.40 | 4od4 | 650.6 | 0 | 0.05 |
| 4p08 | 1192.2 | 39 | 0.53 | 4of5 | 565.9 | 0 | 0.05 |
| 4p12 | 1514.5 | 37 | 0.51 | 4oj0 | 1524.5 | 139 | 0.88 |
| 4p6l | 535.0 | 1 | 0.06 | 4os0 | 1024.8 | 452 | 1.00 |
| 4pu7 | 1034.3 | 282 | 1.00 | 4oyl | 381.5 | 0 | 0.05 |
| 4pus | 653.0 | 0 | 0.05 | 4oyy | 539.1 | 0 | 0.05 |
| 4q9b | 727.8 | 140 | 0.88 | 4p0f | 1184.7 | 19 | 0.32 |
| 4r27 | 890.3 | 0 | 0.05 | 4p0m | 844.4 | 5 | 0.12 |
| 4ra8 | 670.7 | 2 | 0.08 | 4p39 | 783.3 | 22 | 0.35 |
| 4rd9 | 1799.3 | 77 | 0.77 | 4p7o | 1213.8 | 3 | 0.09 |
| 4rdj | 1762.0 | 90 | 0.81 | 4pa1 | 1179.0 | 57 | 0.66 |
| 4ryj | 476.7 | 0 | 0.05 | 4pcf | 657.7 | 0 | 0.05 |
| 4s03 | 851.7 | 49 | 0.61 | 4pek | 665.9 | 0 | 0.05 |
| 4u3q | 651.0 | 0 | 0.05 | 4pgs | 644.6 | 0 | 0.05 |
| 4u4i | 925.8 | 11 | 0.21 | 4pn7 | 702.5 | 0 | 0.05 |
| 4u5h | 590.7 | 11 | 0.21 | 4ppj | 977.6 | 0 | 0.05 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4u64 | 1516.7 | 129 | 0.87 | 4pqz | 377.1 | 0 | 0.05 |
| 4uvj | 1053.6 | 13 | 0.24 | 4psf | 595.2 | 8 | 0.17 |
| 4v1p | 637.6 | 187 | 0.91 | 4pug | 826.8 | 0 | 0.05 |
| 4w6g | 903.5 | 138 | 0.88 | 4pwq | 802.1 | 1 | 0.06 |
| 4w6k | 770.7 | 78 | 0.77 | 4q5y | 1028.2 | 8 | 0.17 |
| 4wnz | 1286.8 | 53 | 0.64 | 4q6z | 625.4 | 0 | 0.05 |
| 4xoh | 1083.9 | 6 | 0.14 | 4q9p | 775.3 | 58 | 0.67 |
| 4zqa | 1794.3 | 58 | 0.67 | 4qcj | 472.0 | 14 | 0.25 |
| 5a2n | 1096.1 | 0 | 0.05 | 4qgy | 573.2 | 0 | 0.05 |
| 5a48 | 778.2 | 1 | 0.06 | 4r7v | 757.5 | 4 | 0.11 |
| | | | | 4rdp | 1381.7 | 111 | 0.85 |
| | | | | 4rid | 1471.5 | 4 | 0.11 |
| | | | | 4rl9 | 506.7 | 0 | 0.05 |
| | | | | 4rln | 568.5 | 0 | 0.05 |
| | | | | 4rs6 | 869.0 | 122 | 0.87 |
| | | | | 4rwi | 1184.5 | 55 | 0.65 |
| | | | | 4tks | 1025.6 | 43 | 0.56 |
| | | | | 4tr5 | 1340.3 | 222 | 1.00 |
| | | | | 4tse | 1057.9 | 26 | 0.40 |
| | | | | 4u2n | 698.3 | 224 | 1.00 |
| | | | | 4u48 | 4122.1 | 21 | 0.34 |
| | | | | 4u9q | 724.9 | 28 | 0.42 |
| | | | | 4ud5 | 886.9 | 0 | 0.05 |
| | | | | 4uex | 709.7 | 0 | 0.05 |
| | | | | 4uu4 | 881.4 | 17 | 0.29 |
| | | | | 4uz2 | 739.0 | 5 | 0.12 |
| | | | | 4w5x | 437.2 | 18 | 0.30 |
| | | | | 4w60 | 399.3 | 37 | 0.51 |
| | | | | 4w8w | 1381.4 | 116 | 0.86 |
| | | | | 4wau | 818.2 | 16 | 0.28 |
| | | | | 4wj2 | 595.3 | 0 | 0.05 |
| | | | | 4wmg | 599.5 | 0 | 0.05 |
| | | | | 4woy | 1029.5 | 44 | 0.57 |
| | | | | 4wz0 | 701.2 | 48 | 0.60 |
| | | | | 4x2w | 1095.6 | 44 | 0.57 |
| | | | | 4x43 | 643.0 | 0 | 0.05 |
| | | | | 4x8h | 974.2 | 6 | 0.14 |
| | | | | 4ynw | 651.0 | 246 | 1.00 |
| | | | | 5bth | 695.4 | 12 | 0.22 |
| | | | | 5c00 | 915.8 | 149 | 0.88 |
| Average | 994.3 | 67.2 | 0.52 | Average | 934.1 | 47.1 | 0.40 |
| Std Dev | 391.7 | 81.5 | 0.31 | Std Dev | 618.9 | 75.5 | 0.30 |

[a] Subset of the test set in Table S9, containing only proteins results from EPPIC and PISA are conflicting, thus one considers the dimer biological the other crystallographic, or the classification by PISA is uncertain.

**Table S13.** Classification of difficult set dimers by three methods[a,b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 3w66 | 0.12 | xtal | dimer | uncertain |
| 3w8g | 0.87 | xtal | dimer | stable |
| 3wtz | 0.74 | xtal | dimer | stable |
| 3wx4 | 0.84 | xtal | dimer | stable |
| 3wyd | 0.72 | xtal | dimer | stable |
| 4chk | 0.62 | bio | monomer | stable |
| 4ckn | 0.77 | xtal | dimer | stable |
| 4cop | 0.83 | xtal | dimer | uncertain |
| 4cw9 | 0.12 | xtal | dimer | stable |
| 4cwc | 0.64 | bio | tetramer | stable |
| 4d28 | 0.51 | xtal | dimer | stable |
| 4jgm | 0.12 | bio | dimer | uncertain |
| 4jup | 0.38 | xtal | dimer | uncertain |
| 4ke2 | 0.18 | xtal | hexamer | stable |
| 4km3 | 0.83 | xtal | dimer | stable |
| 4kp2 | 0.57 | bio | dimer | stable |
| 4l2w | 0.61 | xtal | tetramer | stable |
| 4lft | 0.12 | bio | monomer | stable |
| 4m0q | 0.77 | xtal | dimer | stable |
| 4m23 | 0.78 | bio | dimer | stable |
| 4mdu | 0.19 | xtal | dimer | stable |
| 4nj0 | 1.00 | xtal | dimer | stable |
| 4nqf | 0.49 | xtal | dimer | stable |
| 4nsr | 0.83 | xtal | dimer | stable |
| 4ny0 | 0.12 | xtal | dimer | stable |
| 4o2h | 0.38 | xtal | dimer | stable |
| 4oaf | 0.46 | bio | monomer | stable |
| 4oky | 0.44 | xtal | dimer | stable |
| 4p08 | 0.55 | xtal | dimer | stable |
| 4p12 | 0.54 | bio | dimer | stable |
| 4p6l | 0.13 | xtal | dimer | stable |
| 4pu7 | 1.00 | xtal | dimer | stable |
| 4pus | 0.12 | xtal | dimer | uncertain |
| 4q9b | 0.83 | xtal | dimer | stable |
| 4r27 | 0.12 | bio | monomer | stable |
| 4ra8 | 0.15 | xtal | dimer | stable |
| 4rd9 | 0.75 | bio | dimer | stable |
| 4rdj | 0.79 | xtal | dimer | stable |
| 4ryj | 0.12 | xtal | dimer | stable |
| 4s03 | 0.62 | xtal | dimer | uncertain |
| 4to7 | 1.00 | xtal | monomer | stable |
| 4tqj | 1.00 | xtal | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4u3q | 0.12 | xtal | dimer | uncertain |
| 4u4i | 0.27 | bio | monomer | stable |
| 4u5h | 0.27 | xtal | dimer | stable |
| 4u64 | 0.83 | xtal | dimer | stable |
| 4uvj | 0.29 | xtal | dimer | stable |
| 4v1p | 0.87 | xtal | dimer | stable |
| 4w6g | 0.83 | bio | monomer | stable |
| 4w6k | 0.76 | xtal | dimer | uncertain |
| 4wnz | 0.65 | bio | monomer | stable |
| 4xoh | 0.20 | bio | dimer | stable |
| 4zbw | 0.12 | xtal | monomer | stable |
| 4zqa | 0.68 | xtal | dimer | stable |
| 5a2n | 0.12 | xtal | dimer | stable |
| 5a48 | 0.13 | bio | dimer | uncertain |

[a] Yellow: incorrect classification
[b] Criteria for the selection of the “difficult” subset are given in Table S12

**Table S14.** Classification of test set monomers by three methods[a,b]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 3w9g | 0.23 | xtal | dimer | stable |
| 3wea | 0.12 | xtal | dimer | stable |
| 3wp9 | 0.41 | xtal | dimer | stable |
| 3wpj | 0.12 | bio | monomer | stable |
| 4c41 | 0.12 | bio | monomer | stable |
| 4cbm | 0.12 | bio | dimer | uncertain |
| 4cfi | 0.12 | bio | monomer | stable |
| 4chj | 0.83 | xtal | tetramer | uncertain |
| 4d5r | 0.81 | bio | dimer | stable |
| 4k51 | 0.12 | xtal | trimer | stable |
| 4l8i | 0.12 | xtal | dimer | stable |
| 4l9h | 0.78 | bio | monomer | stable |
| 4lcm | 0.12 | xtal | dimer | stable |
| 4lhf | 0.83 | bio | monomer | stable |
| 4lk4 | 0.24 | bio | monomer | stable |
| 4lso | 0.12 | bio | monomer | stable |
| 4m7g | 0.12 | bio | monomer | stable |
| 4mfi | 0.38 | bio | monomer | stable |
| 4n3x | 0.82 | xtal | tetramer | stable |
| 4n40 | 0.12 | xtal | trimer | stable |
| 4n7f | 0.83 | xtal | dimer | stable |
| 4n8h | 0.53 | bio | monomer | stable |
| 4nl7 | 0.12 | xtal | dimer | stable |
| 4npf | 0.86 | bio | dimer | uncertain |
| 4nv8 | 0.74 | xtal | dimer | stable |
| 4nx9 | 0.68 | bio | monomer | stable |
| 4o6x | 0.83 | xtal | dimer | uncertain |
| 4od4 | 0.12 | xtal | dimer | stable |
| 4of5 | 0.12 | bio | monomer | stable |
| 4oj0 | 0.83 | xtal | dimer | stable |
| 4os0 | 1.00 | xtal | dimer | stable |
| 4oyl | 0.12 | xtal | trimer | uncertain |
| 4oyy | 0.12 | xtal | trimer | stable |
| 4p0f | 0.36 | xtal | dimer | stable |
| 4p0m | 0.19 | xtal | hexamer | stable |
| 4p39 | 0.40 | bio | tetramer | stable |
| 4p7o | 0.16 | xtal | dimer | stable |
| 4pa1 | 0.67 | xtal | dimer | stable |
| 4pcf | 0.12 | bio | trimer | uncertain |
| 4pek | 0.12 | bio | monomer | stable |
| 4pgs | 0.12 | xtal | dimer | stable |
| 4pn7 | 0.12 | bio | monomer | stable |
| 4ppj | 0.12 | bio | monomer | stable |

| | | | | |
|---|---|---|---|---|
| 4pqz | 0.12 | xtal | dimer | uncertain |
| 4psf | 0.23 | bio | monomer | stable |
| 4pug | 0.12 | bio | dimer | stable |
| 4pwq | 0.13 | xtal | dimer | uncertain |
| 4q5y | 0.23 | xtal | dimer | stable |
| 4q6z | 0.12 | xtal | dimer | uncertain |
| 4q7m | 0.84 | bio | dimer | stable |
| 4q9p | 0.68 | xtal | tetramer | uncertain |
| 4qcj | 0.31 | bio | monomer | stable |
| 4qgy | 0.12 | bio | monomer | stable |
| 4r7v | 0.18 | bio | dimer | stable |
| 4rdp | 0.82 | bio | monomer | stable |
| 4rid | 0.18 | bio | tetramer | stable |
| 4rl9 | 0.12 | xtal | tetramer | stable |
| 4rln | 0.12 | bio | monomer | stable |
| 4rs6 | 0.82 | bio | hexamer | stable |
| 4rwi | 0.66 | xtal | dimer | stable |
| 4tks | 0.58 | bio | monomer | stable |
| 4tr5 | 1.00 | bio | monomer | stable |
| 4tse | 0.44 | xtal | dimer | stable |
| 4u2n | 1.00 | xtal | dimer | stable |
| 4u48 | 0.39 | bio | monomer | stable |
| 4u9q | 0.46 | xtal | dimer | uncertain |
| 4ud5 | 0.12 | xtal | dimer | stable |
| 4uex | 0.12 | bio | monomer | stable |
| 4uu4 | 0.34 | bio | monomer | stable |
| 4uz2 | 0.19 | xtal | octomer | stable |
| 4w5x | 0.35 | xtal | dimer | stable |
| 4w60 | 0.54 | xtal | dimer | stable |
| 4w8w | 0.82 | bio | monomer | stable |
| 4wau | 0.33 | xtal | dimer | uncertain |
| 4wj2 | 0.12 | bio | monomer | stable |
| 4wmg | 0.12 | bio | monomer | stable |
| 4woy | 0.59 | bio | tetramer | stable |
| 4wz0 | 0.62 | xtal | dimer | stable |
| 4x2w | 0.59 | bio | tetramer | stable |
| 4x43 | 0.12 | bio | monomer | uncertain |
| 4x8h | 0.20 | bio | monomer | stable |
| 4xm4 | 0.76 | bio | dimer | stable |
| 4ynw | 1.00 | bio | dimer | stable |
| 5avh | 0.79 | bio | tetramer | stable |
| 5bth | 0.28 | bio | monomer | stable |
| 5c00 | 0.83 | bio | monomer | stable |

[a] Yellow: incorrect classification
[b] Criteria for the selection of the “difficult” subset are given in Table S12

**Table S15.** Impact of small interface on success rates[a]

| Test set (783) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Dimers | | | | | | | |
| Interface area (Å²) | Cases | ClusPro | ClusPro % | EPPIC | EPPIC % | PISA | PISA % |
| <600 | 17 | 4 | 23.5% | 4 | 23.5% | 4 | 23.5% |
| <800 | 53 | 26 | 49.1% | 20 | 37.7% | 20 | 37.7% |
| <1000 | 88 | 48 | 54.5% | 37 | 42.0% | 34 | 38.6% |
| Monomers | | | | | | | |
| Interface area (Å²) | Cases | ClusPro | ClusPro % | EPPIC | EPPIC % | PISA | PISA % |
| <600 | 183 | 173 | 94.5% | 165 | 90.2% | 172 | 94.0% |
| <800 | 333 | 299 | 89.8% | 294 | 88.3% | 291 | 87.4% |
| <1000 | 399 | 351 | 88.0% | 344 | 86.2% | 335 | 84.0% |
| Total | | | | | | | |
| Interface area (Å²) | Cases | ClusPro | ClusPro % | EPPIC | EPPIC % | PISA | PISA % |
| <600 | 200 | 177 | 88.5% | 169 | 84.5% | 176 | 88.0% |
| <800 | 386 | 325 | 84.2% | 314 | 81.3% | 311 | 80.6% |
| <1000 | 487 | 399 | 81.9% | 381 | 78.2% | 369 | 75.8% |

[b] Criteria for test selection are given in Table S9

**Table S16.** Transitional complexes: Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the Nooren set[a]

| PDB ID | Interface area (Å²) | $N_{nn}$ | Probability (dimer) |
|---|---|---|---|
| 1a15 | 739.9 | 0 | 0.12 |
| 1a78 | 512.7 | 99 | 0.80 |
| 1bbh | 765.0 | 323 | 1.00 |
| 1beb | 552.5 | 112 | 0.82 |
| 1bfs | 685.1 | 267 | 1.00 |
| 1bft | 688.1 | 275 | 1.00 |
| 1bi2 | 894.5 | 123 | 0.82 |
| 1c0w | 862.3 | 96 | 0.80 |
| 1cmi | 883.6 | 43 | 0.58 |
| 1cnt | 981.2 | 62 | 0.70 |
| 1cpq | 599.6 | 0 | 0.12 |
| 1dom | 845.8 | 99 | 0.80 |
| 1edh | 900.3 | 30 | 0.48 |
| 1ikn | 1141.9 | 316 | 1.00 |
| 1nfk | 683.4 | 32 | 0.49 |
| 1ram | 896.2 | 80 | 0.76 |
| 1scf | 828.4 | 13 | 0.29 |
| 1trz | 793.8 | 19 | 0.36 |
| 1vkx | 1068.0 | 83 | 0.77 |
| 2dtr | 876.1 | 164 | 0.84 |
| 2lyn | 946.1 | 33 | 0.50 |
| 3il8 | 918.6 | 33 | 0.50 |
| 5cro | 638.1 | 126 | 0.83 |
| 6cro | 1821.4 | 244 | 1.00 |
| Average | 855.1 | 111.3 | 0.68 |
| Std Dev | 257.9 | 101.3 | 0.27 |

[a] Transitional complexes from Nooren and Thornton [1]

**Table S17.** Biological activity and classification of Nooren set dimers by three methods[a]

| Protein | PDB ID | Biological activity | | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|---|---|---|
| | | Mono-mer | Dimer | | | | |
| Lambda phage cro repressor | 5cro | − | + | 0.83 | xtal | 24-mer | stable |
| | 6cro | | | 1 | bio | nopred | n/a |
| Corynebacterium diphtheria tox repressorc | 1bi2 | − | + | 0.82 | bio | dimer | stable |
| | 2dtr | | | 0.84 | bio | dimer | stable |
| | 1c0w | | | 0.8 | bio | nopred | n/a |
| Mouse nuclear factor κB (NFκB) P50 and P65 | 1bfs | − | + | 1 | bio | monomer | stable |
| | 1bft | | | 1 | bio | monomer | stable |
| | 1ikn | | | 1 | bio | trimer | stable |
| | 1nfk | | | 0.49 | xtal | tetramer | stable |
| | 1ram | | | 0.76 | bio | tetramer | stable |
| | 1vkx | | | 0.77 | bio | tetramer | stable |
| Human interleukin-8 (IL-8), type I | 3il8 | + | + | 0.5 | bio | dimer | stable |
| Human stromal cell-derived factor 1α (SDF1α), type I | 1a15 | + | ? | 0.12 | xtal | dimer | stable |
| Human monocyte chemoattractant protein 1 (MCP-1), type II | 1dom | + | + | 0.8 | xtal | nopred | n/a |
| Human stem cell factor cytokine (SCF) (secreted soluble form) | 1scf | ? | + | 0.29 | bio | tetramer | stable |
| Human ciliary neurotrophic factor (CNTF) | 1cnt | + | ? | 0.7 | xtal | dimer | stable |
| Human insulin | 1trz | + | ? | 0.36 | bio | dodecamer | stable |
| Chromatium vinosum cytochrome c′ type Ie (CVCP) | 1bbh | + | ? | 1 | bio | dimer | stable |
| Rhodobacter capsulatus cytochrome c′ type IIe (RCCP) | 1cpq | + | ? | 0.12 | xtal | monomer | stable |
| Cow β-lactoglobulin | 1beb | + | + | 0.82 | bio | monomer | stable |
| California red abalone sperm lysin | 2lyn | + | + | 0.5 | xtal | tetramer | stable |
| Mouse epithelial cadherin, first two N-terminal extracellular domain (ECAD12) | 1edh | ? | + | 0.48 | bio | monomer | stable |
| Human LC8 light chain subunit of dynein complex | 1cmi | ? | + | 0.58 | bio | tetramer | stable |
| Toad ovary galectin-1 | 1a78 | ? | ? | 0.8 | xtal | dimer | uncertain |

[a] Transitional complexes from Nooren and Thornton [1]

**Table S18.** Classification of the Nooren set dimers by three methods: Summary

| method | pisa | eppic | cluspro |
|---|---|---|---|
| dimers (24) | 17 | 16 | 18 |
| dimers % | 70.8 | 66.7% | 75.0% |

[a] Transitional complexes from Nooren and Thornton [1]

**Table S19.** Transitional complexes: Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the weak homodimer set selected by Dey et al. [2]

| PDB ID | Interface area (Å²) | $N_{nn}$ | Probability (dimer) |
|---|---|---|---|
| 1a15 | 739.9 | 0 | 0.12 |
| 1a45 | 552.5 | 1 | 0.13 |
| 1a78 | 512.7 | 99 | 0.80 |
| 1b8e | 648.1 | 1 | 0.13 |
| 1bbh | 765.0 | 323 | 1.00 |
| 1bfs | 685.1 | 267 | 1.00 |
| 1cbi | 962.9 | 4 | 0.18 |
| 1cnt | 981.2 | 62 | 0.70 |
| 1cxq | 754.5 | 7 | 0.22 |
| 1dok | 969.5 | 141 | 0.83 |
| 1dto | 983.3 | 0 | 0.12 |
| 1dv8 | 405.3 | 0 | 0.12 |
| 1e87 | 866.0 | 163 | 0.84 |
| 1eaj | 675.2 | 0 | 0.12 |
| 1edh | 900.3 | 30 | 0.48 |
| 1eeq | 679.5 | 143 | 0.83 |
| 1erv | 511.7 | 317 | 1.00 |
| 1exz | 846.3 | 4 | 0.18 |
| 1gml | 786.9 | 33 | 0.50 |
| 1h65 | 1292.2 | 172 | 0.85 |
| 1hgx | 1046.1 | 43 | 0.58 |
| 1ihk | 1204.9 | 140 | 0.83 |
| 1ii5 | 1014.6 | 22 | 0.40 |
| 1itv | 644.8 | 75 | 0.75 |
| 1jr9 | 854.4 | 142 | 0.83 |
| 1lwj | 1318.8 | 119 | 0.82 |
| 1neu | 475.2 | 0 | 0.12 |
| 1nrv | 397.6 | 0 | 0.12 |
| 1o7z | 613.5 | 0 | 0.12 |
| 1oal | 754.5 | 98 | 0.80 |
| 1p9y | 1223.9 | 30 | 0.48 |
| 1py9 | 903.7 | 0 | 0.12 |
| 1sj1 | 367.4 | 0 | 0.12 |
| 1tip | 922.3 | 132 | 0.83 |
| 1uq5 | 911.8 | 14 | 0.31 |
| 1zop | 1068.3 | 175 | 0.85 |
| 2dtr | 876.1 | 164 | 0.84 |
| 2lyn | 946.1 | 33 | 0.50 |
| 3bri | 823.7 | 150 | 0.83 |
| 3il8 | 918.6 | 33 | 0.50 |
| 3sdh | 879.3 | 104 | 0.81 |
| 5cro | 638.1 | 126 | 0.83 |
| Average | 817.2 | 80.2 | 0.54 |
| Std Dev | 234.1 | 88.0 | 0.32 |

**Table S20.** Interface area, number of near-native structures, and inferred probability of being a biological dimer for the proteins in the "others" homodimer set by Dey et al. [2]

| PDB ID | Interface area (Å²) | Nnn | Probability (dimer) |
|---|---|---|---|
| 12as | 1878.1 | 156 | 0.84 |
| 1a3c | 989.1 | 173 | 0.85 |
| 1a4i | 1354.6 | 114 | 0.82 |
| 1aa7 | 1093.8 | 46 | 0.60 |
| 1ad3 | 3940.1 | 39 | 0.55 |
| 1ade | 2699.0 | 107 | 0.81 |
| 1af5 | 851.3 | 0 | 0.12 |
| 1afw | 2388.7 | 123 | 0.82 |
| 1ajs | 3436.9 | 74 | 0.74 |
| 1aor | 1209.9 | 19 | 0.36 |
| 1aoz | 1816.2 | 57 | 0.67 |
| 1aq6 | 2220.5 | 176 | 0.86 |
| 1auo | 663.7 | 0 | 0.12 |
| 1b16 | 2518.4 | 176 | 0.86 |
| 1b3a | 733.0 | 200 | 0.91 |
| 1b5e | 2527.4 | 117 | 0.82 |
| 1b67 | 1595.9 | 283 | 1.00 |
| 1b8a | 4375.3 | 103 | 0.81 |
| 1b8j | 3790.5 | 94 | 0.79 |
| 1b8z | 1889.6 | 242 | 1.00 |
| 1b9h | 2858.4 | 125 | 0.83 |
| 1bam | 750.0 | 128 | 0.83 |
| 1bd0 | 3042.4 | 98 | 0.80 |
| 1bdm | 1588.2 | 259 | 1.00 |
| 1bif | 889.7 | 6 | 0.20 |
| 1biq | 3012.6 | 99 | 0.80 |
| 1bis | 1478.5 | 205 | 0.93 |
| 1bk5 | 1055.9 | 6 | 0.20 |
| 1bkp | 2206.0 | 142 | 0.83 |
| 1brw | 1060.5 | 249 | 1.00 |
| 1bsl | 1893.9 | 158 | 0.84 |
| 1bsr | 1895.4 | 277 | 1.00 |
| 1buo | 1927.6 | 165 | 0.84 |
| 1bxg | 1039.6 | 71 | 0.73 |
| 1byf | 844.0 | 104 | 0.81 |
| 1byi | 1398.3 | 223 | 1.00 |
| 1byk | 1514.5 | 76 | 0.75 |
| 1c4k | 6254.2 | 36 | 0.53 |
| 1cd8 | 1025.3 | 178 | 0.86 |
| 1chm | 3230.1 | 70 | 0.73 |
| 1cmb | 1796.3 | 481 | 1.00 |
| 1cnz | 2444.9 | 107 | 0.81 |
| 1coz | 1053.1 | 192 | 0.89 |
| 1csh | 4995.4 | 61 | 0.69 |
| 1ctt | 1933.3 | 134 | 0.83 |

| | | | |
|---|---|---|---|
| 1czj | 741.3 | 7 | 0.22 |
| 1d0c | 2753.6 | 92 | 0.79 |
| 1d2f | 1757.3 | 103 | 0.81 |
| 1d9c | 3633.0 | 82 | 0.77 |
| 1daa | 2301.1 | 181 | 0.86 |
| 1db3 | 1140.6 | 118 | 0.82 |
| 1dbq | 1532.4 | 56 | 0.66 |
| 1dcf | 1057.3 | 70 | 0.73 |
| 1dor | 2196.2 | 130 | 0.83 |
| 1dos | 2333.0 | 145 | 0.83 |
| 1dpg | 2278.7 | 167 | 0.84 |
| 1dqn | 1724.8 | 88 | 0.78 |
| 1dqs | 1604.6 | 87 | 0.78 |
| 1dxg | 709.8 | 340 | 1.00 |
| 1e1z | 1235.7 | 17 | 0.34 |
| 1e4m | 946.6 | 85 | 0.78 |
| 1e58 | 725.7 | 219 | 0.99 |
| 1e6b | 1144.8 | 52 | 0.64 |
| 1e6u | 1499.9 | 87 | 0.78 |
| 1e7n | 811.9 | 247 | 1.00 |
| 1ebh | 1781.7 | 115 | 0.82 |
| 1ecy | 1562.5 | 63 | 0.70 |
| 1elu | 2940.7 | 85 | 0.78 |
| 1ew3 | 1024.9 | 218 | 0.99 |
| 1ex0 | 2414.9 | 52 | 0.64 |
| 1eyv | 1067.3 | 183 | 0.87 |
| 1f3h | 524.5 | 346 | 1.00 |
| 1f6b | 743.7 | 0 | 0.12 |
| 1f89 | 1407.8 | 134 | 0.83 |
| 1fc4 | 4891.9 | 65 | 0.71 |
| 1fg7 | 3227.5 | 73 | 0.74 |
| 1fi4 | 1373.5 | 140 | 0.83 |
| 1fip | 1578.0 | 209 | 0.94 |
| 1fjj | 873.0 | 134 | 0.83 |
| 1fp1 | 4526.7 | 86 | 0.78 |
| 1fp2 | 4159.7 | 80 | 0.76 |
| 1fp5 | 982.5 | 96 | 0.80 |
| 1fro | 3575.0 | 96 | 0.80 |
| 1g5c | 2129.7 | 231 | 1.00 |
| 1g60 | 1926.3 | 141 | 0.83 |
| 1g8l | 2120.0 | 80 | 0.76 |
| 1gd9 | 2637.7 | 154 | 0.84 |
| 1glj | 1588.3 | 258 | 1.00 |
| 1gnw | 1156.5 | 102 | 0.81 |
| 1gqi | 1935.6 | 50 | 0.63 |
| 1gt3 | 2338.9 | 171 | 0.85 |
| 1gta | 1504.9 | 96 | 0.80 |
| 1gte | 11367.4 | 11 | 0.27 |
| 1gu7 | 894.7 | 188 | 0.88 |
| 1gvj | 1194.9 | 120 | 0.82 |
| 1gvp | 905.1 | 192 | 0.89 |
| 1gy6 | 1241.9 | 175 | 0.85 |
| 1gyo | 610.9 | 0 | 0.12 |

| | | | |
|---|---|---|---|
| 1h16 | 1890.0 | 157 | 0.84 |
| 1h1y | 945.2 | 119 | 0.82 |
| 1h4v | 3708.2 | 69 | 0.73 |
| 1h7e | 1361.9 | 173 | 0.85 |
| 1h9r | 1386.3 | 66 | 0.71 |
| 1hf2 | 1041.6 | 208 | 0.94 |
| 1hjr | 962.0 | 83 | 0.77 |
| 1hpx | 1731.3 | 273 | 1.00 |
| 1hq8 | 1016.7 | 151 | 0.83 |
| 1hss | 1095.5 | 64 | 0.70 |
| 1hw1 | 1593.0 | 138 | 0.83 |
| 1hxp | 3398.7 | 113 | 0.82 |
| 1hzj | 976.3 | 188 | 0.88 |
| 1i07 | 1960.6 | 201 | 0.91 |
| 1i24 | 2423.5 | 101 | 0.81 |
| 1i2k | 2225.1 | 175 | 0.85 |
| 1i4u | 1285.5 | 66 | 0.71 |
| 1i52 | 1822.5 | 126 | 0.83 |
| 1i69 | 1069.1 | 58 | 0.68 |
| 1i86 | 2974.1 | 75 | 0.75 |
| 1imb | 1648.7 | 185 | 0.87 |
| 1is3 | 748.3 | 66 | 0.71 |
| 1iup | 987.0 | 153 | 0.83 |
| 1ivy | 1586.2 | 141 | 0.83 |
| 1ix9 | 907.8 | 115 | 0.82 |
| 1iyz | 948.2 | 68 | 0.72 |
| 1j3b | 973.1 | 0 | 0.12 |
| 1j5p | 2146.1 | 172 | 0.85 |
| 1j98 | 1869.9 | 125 | 0.83 |
| 1jd0 | 1121.6 | 0 | 0.12 |
| 1jdw | 1473.4 | 101 | 0.81 |
| 1jhd | 1547.2 | 44 | 0.59 |
| 1jhg | 2225.9 | 349 | 1.00 |
| 1jm6 | 1096.3 | 7 | 0.22 |
| 1jsc | 2200.4 | 113 | 0.82 |
| 1jsg | 789.3 | 146 | 0.83 |
| 1jtv | 2603.8 | 141 | 0.83 |
| 1jye | 1528.6 | 88 | 0.78 |
| 1jys | 1249.1 | 162 | 0.84 |
| 1k04 | 2356.6 | 107 | 0.81 |
| 1k3y | 1405.9 | 104 | 0.81 |
| 1k51 | 2340.5 | 133 | 0.83 |
| 1k66 | 1248.4 | 191 | 0.88 |
| 1k94 | 1820.6 | 272 | 1.00 |
| 1kc7 | 2030.4 | 105 | 0.81 |
| 1kcm | 1510.7 | 148 | 0.83 |
| 1kic | 942.7 | 0 | 0.12 |
| 1kjq | 2304.9 | 99 | 0.80 |
| 1kkj | 3700.6 | 115 | 0.82 |
| 1kll | 2050.8 | 220 | 1.00 |
| 1kly | 1642.4 | 226 | 1.00 |
| 1knq | 1029.8 | 165 | 0.84 |
| 1kpf | 1855.0 | 198 | 0.90 |

| | | | |
|---|---|---|---|
| 1kso | 1680.6 | 291 | 1.00 |
| 1kta | 2339.6 | 159 | 0.84 |
| 1ktb | 989.9 | 2 | 0.15 |
| 1kzh | 2096.1 | 103 | 0.81 |
| 1lc5 | 1943.0 | 231 | 1.00 |
| 1llf | 681.6 | 0 | 0.12 |
| 1lom | 3217.1 | 40 | 0.56 |
| 1lxe | 2444.8 | 61 | 0.69 |
| 1m6p | 1017.7 | 99 | 0.80 |
| 1m7y | 2701.7 | 118 | 0.82 |
| 1mh9 | 1132.0 | 137 | 0.83 |
| 1mkb | 1598.0 | 124 | 0.82 |
| 1mo9 | 4712.5 | 95 | 0.80 |
| 1mor | 2528.4 | 97 | 0.80 |
| 1mqi | 787.9 | 24 | 0.42 |
| 1mr8 | 1289.3 | 387 | 1.00 |
| 1mvc | 1084.3 | 64 | 0.70 |
| 1mze | 1614.9 | 416 | 1.00 |
| 1n1b | 1177.6 | 212 | 0.96 |
| 1n26 | 1112.5 | 3 | 0.16 |
| 1n2s | 1374.1 | 155 | 0.84 |
| 1n55 | 1397.6 | 189 | 0.88 |
| 1n57 | 945.8 | 162 | 0.84 |
| 1n7f | 633.1 | 44 | 0.59 |
| 1nf9 | 1320.5 | 230 | 1.00 |
| 1nkd | 1377.7 | 154 | 0.84 |
| 1nn5 | 769.8 | 232 | 1.00 |
| 1noj | 2540.4 | 79 | 0.76 |
| 1nox | 2966.1 | 122 | 0.82 |
| 1ns5 | 1107.9 | 214 | 0.97 |
| 1nsj | 1420.5 | 326 | 1.00 |
| 1nsy | 2583.3 | 120 | 0.82 |
| 1o8b | 1077.0 | 170 | 0.85 |
| 1oaa | 1932.7 | 137 | 0.83 |
| 1oac | 7135.2 | 16 | 0.33 |
| 1oc2 | 1300.9 | 132 | 0.83 |
| 1oh0 | 1038.7 | 89 | 0.79 |
| 1oi6 | 1646.7 | 139 | 0.83 |
| 1oke | 1929.2 | 12 | 0.28 |
| 1on2 | 1257.2 | 120 | 0.82 |
| 1oqz | 990.0 | 9 | 0.24 |
| 1ov3 | 2449.9 | 143 | 0.83 |
| 1oyb | 735.5 | 44 | 0.59 |
| 1oys | 1387.3 | 127 | 0.83 |
| 1p5f | 1339.3 | 156 | 0.84 |
| 1pfq | 2176.4 | 89 | 0.79 |
| 1pre | 2280.7 | 33 | 0.50 |
| 1psr | 1199.3 | 291 | 1.00 |
| 1puc | 2148.8 | 199 | 0.91 |
| 1pv9 | 1663.1 | 58 | 0.68 |
| 1pxf | 2202.5 | 243 | 1.00 |
| 1q3o | 604.3 | 0 | 0.12 |
| 1q4g | 2503.8 | 30 | 0.48 |

| | | | |
|---|---|---|---|
| 1q6o | 1444.6 | 71 | 0.73 |
| 1qfh | 2275.0 | 55 | 0.66 |
| 1qhi | 1698.8 | 103 | 0.81 |
| 1qi9 | 5330.3 | 36 | 0.53 |
| 1qj4 | 844.8 | 102 | 0.81 |
| 1qjb | 973.9 | 101 | 0.81 |
| 1qkk | 923.9 | 51 | 0.64 |
| 1qks | 1288.6 | 28 | 0.46 |
| 1qo8 | 1233.0 | 22 | 0.40 |
| 1qr2 | 1917.0 | 130 | 0.83 |
| 1qvz | 549.1 | 0 | 0.12 |
| 1qyc | 1146.8 | 300 | 1.00 |
| 1r2f | 1741.9 | 127 | 0.83 |
| 1r31 | 4779.1 | 88 | 0.78 |
| 1r3s | 1233.5 | 78 | 0.76 |
| 1r7a | 958.3 | 103 | 0.81 |
| 1rdo | 663.4 | 294 | 1.00 |
| 1reg | 676.5 | 0 | 0.12 |
| 1rrm | 1153.9 | 95 | 0.80 |
| 1ryt | 1638.5 | 152 | 0.83 |
| 1s0a | 5189.6 | 85 | 0.78 |
| 1s3e | 2042.9 | 23 | 0.41 |
| 1sb8 | 1176.5 | 82 | 0.77 |
| 1se8 | 1097.1 | 19 | 0.36 |
| 1ses | 2229.6 | 107 | 0.81 |
| 1sjy | 1526.2 | 140 | 0.83 |
| 1smn | 868.4 | 164 | 0.84 |
| 1smt | 1969.4 | 278 | 1.00 |
| 1sox | 1410.1 | 87 | 0.78 |
| 1t0i | 1317.6 | 261 | 1.00 |
| 1t5h | 1329.7 | 48 | 0.62 |
| 1tc1 | 1505.7 | 92 | 0.79 |
| 1tox | 3703.5 | 86 | 0.78 |
| 1trb | 2735.2 | 170 | 0.85 |
| 1trk | 4418.3 | 54 | 0.65 |
| 1tw3 | 3376.7 | 177 | 0.86 |
| 1ual | 3517.1 | 110 | 0.82 |
| 1uby | 2162.4 | 135 | 0.83 |
| 1ui8 | 6595.9 | 8 | 0.23 |
| 1ukg | 838.3 | 25 | 0.43 |
| 1utg | 1464.2 | 177 | 0.86 |
| 1uyr | 5132.3 | 10 | 0.26 |
| 1v25 | 2850.8 | 129 | 0.83 |
| 1v2z | 841.3 | 142 | 0.83 |
| 1vfr | 3355.7 | 73 | 0.74 |
| 1vhz | 2820.5 | 148 | 0.83 |
| 1vls | 1254.6 | 44 | 0.59 |
| 1vok | 1582.6 | 159 | 0.84 |
| 1xso | 666.8 | 102 | 0.81 |
| 2arc | 810.3 | 83 | 0.77 |
| 2gsa | 4576.7 | 85 | 0.78 |
| 2hdh | 1604.4 | 260 | 1.00 |
| 2ilk | 4479.7 | 43 | 0.58 |

| | | | |
|---|---|---|---|
| 2mjp | 950.0 | 252 | 1.00 |
| 2nac | 3793.4 | 180 | 0.86 |
| 2ohx | 1685.1 | 339 | 1.00 |
| 2spc | 2513.5 | 57 | 0.67 |
| 2tct | 2612.3 | 137 | 0.83 |
| 2tgi | 1260.4 | 145 | 0.83 |
| 3dap | 2653.4 | 154 | 0.84 |
| 3lad | 3364.1 | 120 | 0.82 |
| 3ssi | 838.4 | 115 | 0.82 |
| 3vub | 1003.5 | 296 | 1.00 |
| 4kbp | 1467.9 | 125 | 0.83 |
| 5csm | 2000.1 | 38 | 0.54 |
| 5rub | 2829.1 | 99 | 0.80 |
| 8prk | 968.0 | 239 | 1.00 |
| 9wga | 2298.4 | 151 | 0.83 |
| Average | 1922.8 | 125.9 | 0.75 |
| Std Dev | 1260.2 | 83.2 | 0.22 |

**Table S21**. Classification of the weak set of dimers by Dey et al. [2]

| PDB ID | Kd (μM) | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|---|
| 1a15 | 150 | 0.12 | xtal | dimer | stable |
| 1a45 | — | 0.13 | xtal | monomer | stable |
| 1a78 | 7 | 0.80 | xtal | dimer | uncertain |
| 1b8e | 5–200 | 0.13 | bio | monomer | stable |
| 1bbh | 2000 | 1.00 | bio | dimer | stable |
| 1bfs | 0.7 | 1.00 | bio | monomer | stable |
| 1cbi | > 100 | 0.18 | xtal | dimer | stable |
| 1cnt | ≈ 40 | 0.70 | xtal | dimer | stable |
| 1cxq | 10–50 | 0.22 | bio | dimer | stable |
| 1dok | 1–10 | 0.83 | xtal | tetramer | stable |
| 1dto | 0.03 | 0.12 | xtal | monomer | stable |
| 1dv8 | — | 0.12 | xtal | dimer | stable |
| 1e87 | — | 0.84 | xtal | monomer | stable |
| 1eaj | 16 | 0.12 | bio | dimer | stable |
| 1edh | 170–720 | 0.48 | bio | monomer | stable |
| 1eeq | 0.012 | 0.83 | xtal | dimer | stable |
| 1erv | 6–160 | 1.00 | bio | dimer | uncertain |
| 1exz | < 0.1 | 0.18 | bio | tetramer | stable |
| 1gml | — | 0.50 | bio | dimer | uncertain |
| 1h65 | — | 0.85 | xtal | dimer | stable |
| 1hgx | — | 0.58 | xtal | dimer | stable |
| 1ihk | 0.7 | 0.83 | xtal | dimer | stable |
| 1ii5 | 0.8 | 0.40 | bio | dimer | uncertain |
| 1itv | — | 0.75 | bio | monomer | stable |
| 1jr9 | — | 0.83 | bio | dimer | stable |
| 1lwj | — | 0.82 | bio | dimer | stable |
| 1neu | 900 | 0.12 | xtal | monomer | stable |
| 1nrv | 2 | 0.12 | xtal | monomer | stable |
| 1o7z | 9 | 0.12 | xtal | dimer | stable |
| 1oal | 0.3 | 0.80 | bio | dimer | stable |
| 1p9y | 18 | 0.48 | bio | monomer | stable |
| 1py9 | — | 0.12 | bio | dimer | stable |
| 1sj1 | — | 0.12 | xtal | monomer | stable |
| 1tip | — | 0.83 | xtal | monomer | stable |
| 1uq5 | — | 0.31 | xtal | dimer | stable |
| 1zop | — | 0.85 | bio | dimer | stable |
| 2dtr | 0.033 | 0.84 | bio | dimer | stable |
| 2lyn | ≈ 1 | 0.50 | xtal | tetramer | stable |
| 3bri | 12 | 0.83 | bio | dimer | stable |
| 3il8 | 0.3–18 | 0.50 | bio | dimer | stable |
| 3sdh | 0.013 | 0.81 | bio | dimer | stable |
| 5cro | 0.3 | 0.83 | xtal | 24-mer | stable |

**Table S22**. Classification of the “others” set of dimers by Dey et al. [2]

| PDB ID | ClusPro probability of dimer | EPPIC | PISA multimer class | PISA status |
|---|---|---|---|---|
| 12as | 0.84 | bio | dimer | stable |
| 1a3c | 0.85 | bio | dimer | stable |
| 1a4i | 0.82 | bio | dimer | stable |
| 1aa7 | 0.60 | bio | monomer | stable |
| 1ad3 | 0.55 | bio | dimer | stable |
| 1ade | 0.81 | bio | dimer | stable |
| 1af5 | 0.12 | bio | dimer | stable |
| 1afw | 0.82 | bio | dimer | stable |
| 1ajs | 0.74 | bio | dimer | stable |
| 1aor | 0.36 | bio | dimer | stable |
| 1aoz | 0.67 | xtal | tetramer | stable |
| 1aq6 | 0.86 | bio | dimer | stable |
| 1auo | 0.12 | bio | dimer | stable |
| 1b16 | 0.86 | bio | dimer | stable |
| 1b3a | 0.91 | bio | dimer | stable |
| 1b5e | 0.82 | bio | dimer | stable |
| 1b67 | 1.00 | xtal | dimer | stable |
| 1b8a | 0.81 | bio | dimer | stable |
| 1b8j | 0.79 | bio | dimer | stable |
| 1b8z | 1.00 | bio | dimer | stable |
| 1b9h | 0.83 | bio | dimer | stable |
| 1bam | 0.83 | xtal | dimer | uncertain |
| 1bd0 | 0.80 | bio | dimer | stable |
| 1bdm | 1.00 | bio | dimer | stable |
| 1bif | 0.20 | xtal | monomer | stable |
| 1biq | 0.80 | bio | dimer | stable |
| 1bis | 0.93 | bio | dimer | stable |
| 1bk5 | 0.20 | bio | monomer | stable |
| 1bkp | 0.83 | bio | dimer | stable |
| 1brw | 1.00 | bio | dimer | stable |
| 1bsl | 0.84 | bio | dimer | stable |
| 1bsr | 1.00 | bio | tetramer | stable |
| 1buo | 0.84 | bio | dimer | stable |
| 1bxg | 0.73 | bio | dimer | uncertain |
| 1byf | 0.81 | bio | dimer | stable |
| 1byi | 1.00 | bio | dimer | stable |
| 1byk | 0.75 | bio | dimer | stable |
| 1c4k | 0.53 | bio | dimer | stable |
| 1cd8 | 0.86 | bio | dimer | stable |
| 1chm | 0.73 | bio | dimer | stable |
| 1cmb | 1.00 | bio | dimer | stable |
| 1cnz | 0.81 | bio | dimer | stable |
| 1coz | 0.89 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1csh | 0.69 | bio | dimer | stable |
| 1ctt | 0.83 | bio | dimer | stable |
| 1czj | 0.22 | bio | dimer | stable |
| 1d0c | 0.79 | bio | dimer | stable |
| 1d2f | 0.81 | bio | dimer | stable |
| 1d9c | 0.77 | bio | dimer | stable |
| 1daa | 0.86 | bio | dimer | stable |
| 1db3 | 0.82 | bio | hexamer | stable |
| 1dbq | 0.66 | bio | dimer | stable |
| 1dcf | 0.73 | bio | dimer | stable |
| 1dor | 0.83 | bio | dimer | stable |
| 1dos | 0.83 | bio | dimer | stable |
| 1dpg | 0.84 | bio | dimer | stable |
| 1dqn | 0.78 | bio | dimer | stable |
| 1dqs | 0.78 | bio | dimer | stable |
| 1dxg | 1.00 | bio | dimer | stable |
| 1e1z | 0.34 | bio | octomer | stable |
| 1e4m | 0.78 | bio | dimer | stable |
| 1e58 | 0.99 | xtal | dimer | stable |
| 1e6b | 0.64 | xtal | dimer | stable |
| 1e6u | 0.78 | bio | dimer | stable |
| 1e7n | 1.00 | bio | dimer | uncertain |
| 1ebh | 0.82 | bio | dimer | stable |
| 1ecy | 0.70 | bio | monomer | stable |
| 1elu | 0.78 | bio | dimer | stable |
| 1ew3 | 0.99 | xtal | dimer | stable |
| 1ex0 | 0.64 | bio | dimer | stable |
| 1eyv | 0.87 | xtal | dimer | stable |
| 1f3h | 1.00 | xtal | dimer | stable |
| 1f6b | 0.12 | xtal | monomer | stable |
| 1f89 | 0.83 | bio | dimer | stable |
| 1fc4 | 0.71 | bio | dimer | stable |
| 1fg7 | 0.74 | bio | dimer | stable |
| 1fi4 | 0.83 | bio | dimer | stable |
| 1fip | 0.94 | bio | tetramer | stable |
| 1fjj | 0.83 | bio | monomer | stable |
| 1fp1 | 0.78 | bio | dimer | stable |
| 1fp2 | 0.76 | bio | dimer | stable |
| 1fp5 | 0.80 | bio | dimer | stable |
| 1fro | 0.80 | bio | dimer | stable |
| 1g5c | 1.00 | bio | dimer | stable |
| 1g60 | 0.83 | bio | dimer | stable |
| 1g8l | 0.76 | xtal | dimer | stable |
| 1gd9 | 0.84 | bio | dimer | stable |
| 1glj | 1.00 | bio | dimer | stable |
| 1gnw | 0.81 | bio | dimer | stable |
| 1gqi | 0.63 | bio | monomer | stable |
| 1gt3 | 0.85 | bio | dimer | stable |
| 1gta | 0.80 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1gte | 0.27 | bio | dimer | stable |
| 1gu7 | 0.88 | bio | dimer | stable |
| 1gvj | 0.82 | xtal | dimer | stable |
| 1gvp | 0.89 | bio | dimer | stable |
| 1gy6 | 0.85 | bio | dimer | stable |
| 1gyo | 0.12 | xtal | dimer | stable |
| 1h16 | 0.84 | bio | dimer | stable |
| 1h1y | 0.82 | bio | dimer | stable |
| 1h4v | 0.73 | bio | dimer | stable |
| 1h7e | 0.85 | bio | dimer | stable |
| 1h9r | 0.71 | bio | nopred | n/a |
| 1hf2 | 0.94 | bio | tetramer | stable |
| 1hjr | 0.77 | bio | dimer | stable |
| 1hpx | 1.00 | bio | dimer | stable |
| 1hq8 | 0.83 | xtal | dimer | uncertain |
| 1hss | 0.70 | bio | dimer | stable |
| 1hw1 | 0.83 | bio | dimer | stable |
| 1hxp | 0.82 | bio | dimer | stable |
| 1hzj | 0.88 | bio | dimer | stable |
| 1i07 | 0.91 | bio | dimer | stable |
| 1i24 | 0.81 | bio | tetramer | stable |
| 1i2k | 0.85 | bio | dimer | stable |
| 1i4u | 0.71 | xtal | dimer | stable |
| 1i52 | 0.83 | bio | dimer | stable |
| 1i69 | 0.68 | bio | dimer | stable |
| 1i86 | 0.75 | bio | dimer | stable |
| 1imb | 0.87 | xtal | dimer | stable |
| 1is3 | 0.71 | bio | dimer | uncertain |
| 1iup | 0.83 | bio | monomer | stable |
| 1ivy | 0.83 | bio | dimer | stable |
| 1ix9 | 0.82 | xtal | dimer | stable |
| 1iyz | 0.72 | bio | dimer | stable |
| 1j3b | 0.12 | bio | dimer | stable |
| 1j5p | 0.85 | bio | dimer | stable |
| 1j98 | 0.83 | bio | dimer | stable |
| 1jd0 | 0.12 | xtal | monomer | stable |
| 1jdw | 0.81 | bio | dimer | stable |
| 1jhd | 0.59 | bio | dimer | stable |
| 1jhg | 1.00 | bio | dimer | stable |
| 1jm6 | 0.22 | bio | dimer | stable |
| 1jsc | 0.82 | bio | dimer | stable |
| 1jsg | 0.83 | bio | tetramer | stable |
| 1jtv | 0.83 | bio | dimer | stable |
| 1jye | 0.78 | bio | dimer | stable |
| 1jys | 0.84 | bio | dimer | stable |
| 1k04 | 0.81 | bio | dimer | stable |
| 1k3y | 0.81 | bio | dimer | stable |
| 1k51 | 0.83 | bio | dimer | stable |
| 1k66 | 0.88 | xtal | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1k94 | 1.00 | bio | dimer | stable |
| 1kc7 | 0.81 | bio | dimer | stable |
| 1kcm | 0.83 | bio | dimer | stable |
| 1kic | 0.12 | bio | dimer | stable |
| 1kjq | 0.80 | bio | dimer | stable |
| 1kkj | 0.82 | bio | dimer | stable |
| 1kll | 1.00 | xtal | dimer | stable |
| 1kly | 1.00 | bio | dimer | stable |
| 1knq | 0.84 | bio | dimer | uncertain |
| 1kpf | 0.90 | bio | dimer | stable |
| 1kso | 1.00 | bio | dimer | stable |
| 1kta | 0.84 | bio | dimer | stable |
| 1ktb | 0.15 | bio | dimer | stable |
| 1kzh | 0.81 | bio | dimer | stable |
| 1lc5 | 1.00 | bio | dimer | stable |
| 1llf | 0.12 | xtal | dimer | stable |
| 1lom | 0.56 | bio | dimer | stable |
| 1lxe | 0.69 | bio | dimer | stable |
| 1m6p | 0.80 | bio | dimer | stable |
| 1m7y | 0.82 | bio | dimer | stable |
| 1mh9 | 0.83 | bio | dimer | stable |
| 1mkb | 0.82 | bio | dimer | stable |
| 1mo9 | 0.80 | bio | dimer | stable |
| 1mor | 0.80 | bio | dimer | stable |
| 1mqi | 0.42 | xtal | dimer | uncertain |
| 1mr8 | 1.00 | bio | tetramer | stable |
| 1mvc | 0.70 | bio | dimer | stable |
| 1mze | 1.00 | bio | dimer | stable |
| 1n1b | 0.96 | xtal | dimer | stable |
| 1n26 | 0.16 | xtal | dimer | stable |
| 1n2s | 0.84 | bio | dimer | stable |
| 1n55 | 0.88 | bio | dimer | stable |
| 1n57 | 0.84 | bio | dimer | stable |
| 1n7f | 0.59 | xtal | tetramer | stable |
| 1nf9 | 1.00 | bio | dimer | stable |
| 1nkd | 0.84 | bio | dimer | stable |
| 1nn5 | 1.00 | bio | dimer | stable |
| 1noj | 0.76 | bio | dimer | stable |
| 1nox | 0.82 | bio | dimer | stable |
| 1ns5 | 0.97 | bio | dimer | stable |
| 1nsj | 1.00 | bio | dimer | stable |
| 1nsy | 0.82 | bio | dimer | stable |
| 1o8b | 0.85 | xtal | dimer | stable |
| 1oaa | 0.83 | bio | dimer | stable |
| 1oac | 0.33 | bio | dimer | stable |
| 1oc2 | 0.83 | bio | dimer | stable |
| 1oh0 | 0.79 | bio | dimer | stable |
| 1oi6 | 0.83 | bio | dimer | stable |
| 1oke | 0.28 | xtal | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1on2 | 0.82 | bio | dimer | stable |
| 1oqz | 0.24 | xtal | monomer | stable |
| 1ov3 | 0.83 | bio | octomer | stable |
| 1oyb | 0.59 | bio | monomer | stable |
| 1oys | 0.83 | bio | dimer | uncertain |
| 1p5f | 0.84 | bio | dimer | stable |
| 1pfq | 0.79 | bio | dimer | stable |
| 1pre | 0.50 | bio | dimer | stable |
| 1psr | 1.00 | bio | dimer | stable |
| 1puc | 0.91 | bio | dimer | stable |
| 1pv9 | 0.68 | bio | dimer | stable |
| 1pxf | 1.00 | bio | dimer | stable |
| 1q3o | 0.12 | xtal | dimer | stable |
| 1q4g | 0.48 | bio | dimer | stable |
| 1q6o | 0.73 | bio | tetramer | stable |
| 1qfh | 0.66 | bio | dimer | stable |
| 1qhi | 0.81 | bio | dimer | stable |
| 1qi9 | 0.53 | bio | dimer | stable |
| 1qj4 | 0.81 | xtal | dimer | stable |
| 1qjb | 0.81 | bio | tetramer | stable |
| 1qkk | 0.64 | bio | tetramer | stable |
| 1qks | 0.46 | bio | dimer | stable |
| 1qo8 | 0.40 | bio | monomer | stable |
| 1qr2 | 0.83 | bio | dimer | stable |
| 1qvz | 0.12 | xtal | monomer | stable |
| 1qyc | 1.00 | xtal | dimer | stable |
| 1r2f | 0.83 | bio | dimer | stable |
| 1r31 | 0.78 | bio | hexamer | stable |
| 1r3s | 0.76 | bio | dimer | stable |
| 1r7a | 0.81 | bio | dimer | uncertain |
| 1rdo | 1.00 | xtal | dimer | stable |
| 1reg | 0.12 | bio | dimer | stable |
| 1rrm | 0.80 | bio | dimer | stable |
| 1ryt | 0.83 | bio | tetramer | stable |
| 1s0a | 0.78 | bio | dimer | stable |
| 1s3e | 0.41 | bio | dimer | stable |
| 1sb8 | 0.77 | bio | dimer | stable |
| 1se8 | 0.36 | bio | dimer | stable |
| 1ses | 0.81 | bio | dimer | stable |
| 1sjy | 0.83 | bio | dimer | stable |
| 1smn | 0.84 | xtal | dimer | uncertain |
| 1smt | 1.00 | bio | dimer | stable |
| 1sox | 0.78 | bio | dimer | stable |
| 1t0i | 1.00 | bio | tetramer | stable |
| 1t5h | 0.62 | bio | monomer | stable |
| 1tc1 | 0.79 | bio | dimer | stable |
| 1tox | 0.78 | bio | dimer | stable |
| 1trb | 0.85 | bio | dimer | stable |
| 1trk | 0.65 | bio | dimer | stable |

| | | | | |
|---|---|---|---|---|
| 1tw3 | 0.86 | bio | dimer | stable |
| 1ual | 0.82 | bio | dimer | stable |
| 1uby | 0.83 | bio | dimer | stable |
| 1ui8 | 0.23 | bio | dimer | stable |
| 1ukg | 0.43 | xtal | dimer | uncertain |
| 1utg | 0.86 | bio | dimer | stable |
| 1uyr | 0.26 | bio | dimer | stable |
| 1v25 | 0.83 | bio | dimer | stable |
| 1v2z | 0.83 | bio | dimer | stable |
| 1vfr | 0.74 | bio | dimer | stable |
| 1vhz | 0.83 | bio | dimer | stable |
| 1vls | 0.59 | bio | dimer | stable |
| 1vok | 0.84 | bio | tetramer | stable |
| 1xso | 0.81 | bio | dimer | stable |
| 2arc | 0.77 | bio | monomer | stable |
| 2gsa | 0.78 | bio | dimer | stable |
| 2hdh | 1.00 | bio | dimer | stable |
| 2ilk | 0.58 | bio | dimer | stable |
| 2mjp | 1.00 | bio | dimer | stable |
| 2nac | 0.86 | bio | dimer | stable |
| 2ohx | 1.00 | xtal | dimer | stable |
| 2spc | 0.67 | bio | dimer | stable |
| 2tct | 0.83 | bio | dimer | stable |
| 2tgi | 0.83 | bio | dimer | stable |
| 3dap | 0.84 | bio | dimer | stable |
| 3lad | 0.82 | bio | dimer | stable |
| 3ssi | 0.82 | bio | dimer | stable |
| 3vub | 1.00 | bio | dimer | stable |
| 4kbp | 0.83 | bio | tetramer | stable |
| 5csm | 0.54 | bio | dimer | stable |
| 5rub | 0.80 | bio | dimer | stable |
| 8prk | 1.00 | bio | dimer | stable |
| 9wga | 0.83 | bio | dimer | stable |

**Table S23.** Classification of the weak set of dimers by Dey et al. [2] using three methods: Summary

| method | pisa | eppic | cluspro |
|---|---|---|---|
| dimers (42) | 22 | 21 | 24 |
| dimers % | 52.4% | 50.0% | 57.1% |

**Table S24.** Classification of the “others” set of dimers by Dey et al. [2] using three methods: Summary

| method | pisa | eppic | cluspro |
|---|---|---|---|
| dimers (272) | 226 | 236 | 240 |
| dimers % | 83.1% | 86.8% | 88.2% |

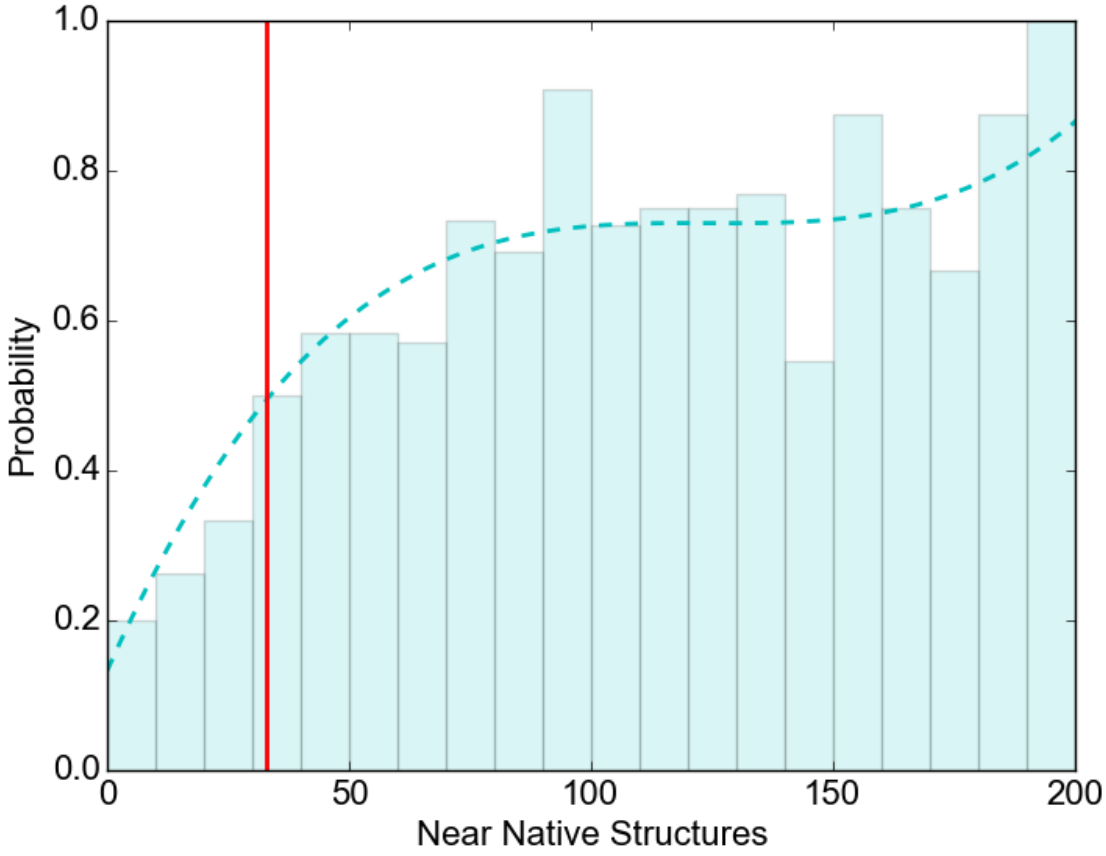



**Figure S1.**

**Figure S1.** Probability of biological dimer for combined training and test sets

**Figure S2.** (Page 12) Analysis of CAPRI target T70 (Modulator protein MzrA, PDB ID 4pwu). **(a)** Input for the analysis of the interface between chains A and B. **(b)** Status page showing the input and processed PDB files.

**Figure S3.** (Page 13) Results of the analysis of the interaction between chains A and B in CAPRI target T70 (Modulator protein MzrA, PDB ID 4pwu). **(a)** The result page shows the number $N_{nn}$ of near-native docked structures among the lowest energy 1000 structures, indicated by a vertical red line, and the implied probability of the interface being in a biological dimer. Since for this dimer $N_{nn}$ = 214, it is off the scale of the figure . Note the label for downloading the PyMOL session at the bottom of the page. **(b)** The PyMOL session downloaded shows the subunit 1 considered the receptor (solid grey), subunit 2 considered the ligand (solid green), and the top 100 lowest energy structures (green transparent cartoons). A large number but not all overlap with the native ligand positions.

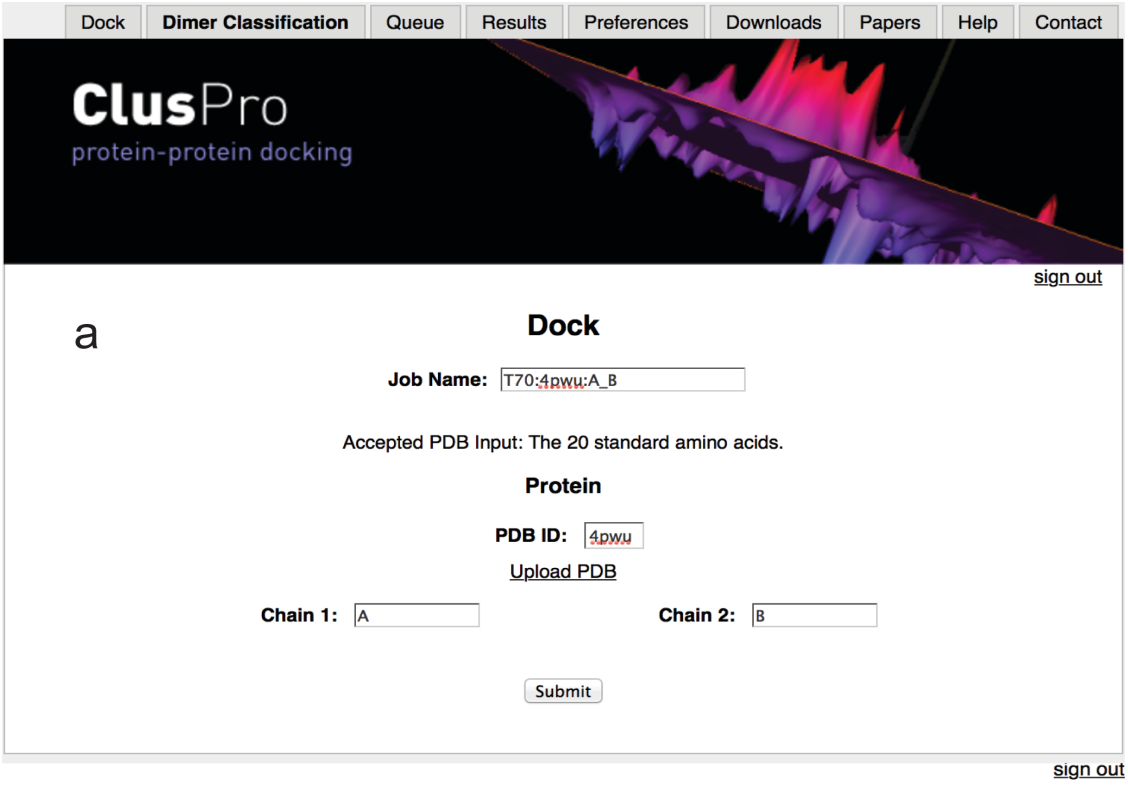
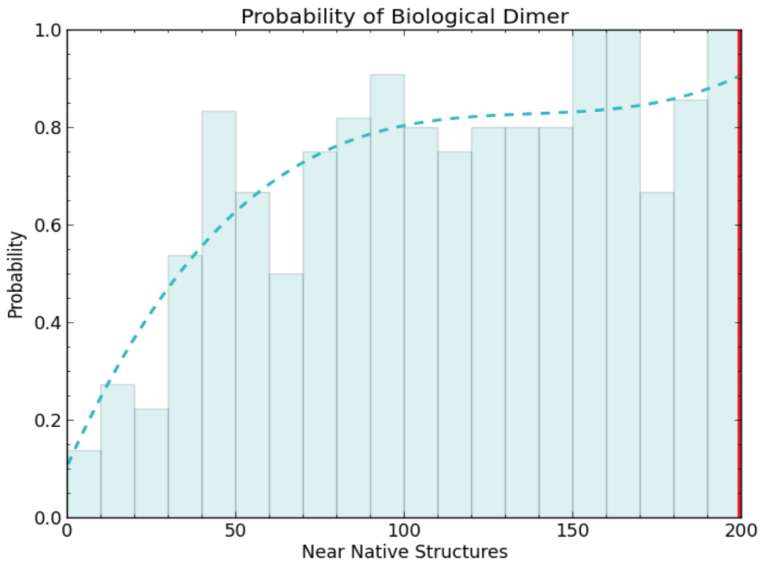

Dock
Dimer Classification
Queue
Results
Preferences
Downloads
Papers
Help
Contact
ClusPro
protein-protein docking
sign out
a
Dock
Job Name:
T70:4pwu:A_B
Accepted PDB Input: The 20 standard amino acids.
Protein
PDB ID:
4pwu
Upload PDB
Chain 1:
A
Chain 2:
B
Submit
sign out
b
171138: T70:4pwu:A_B
Status finished (View Models)
Submitted 2016-06-26 13:40:07
Errors (none reported)
Rotations 70000
user input
rec
lig
chains:
A
chains:
B
processed files
rec
lig

**Figure S2**

a

Result: Likely Biological

**Near-native count:** 214
**Probability of being a biological dimer:** 97%




Download PyMOL Session

b

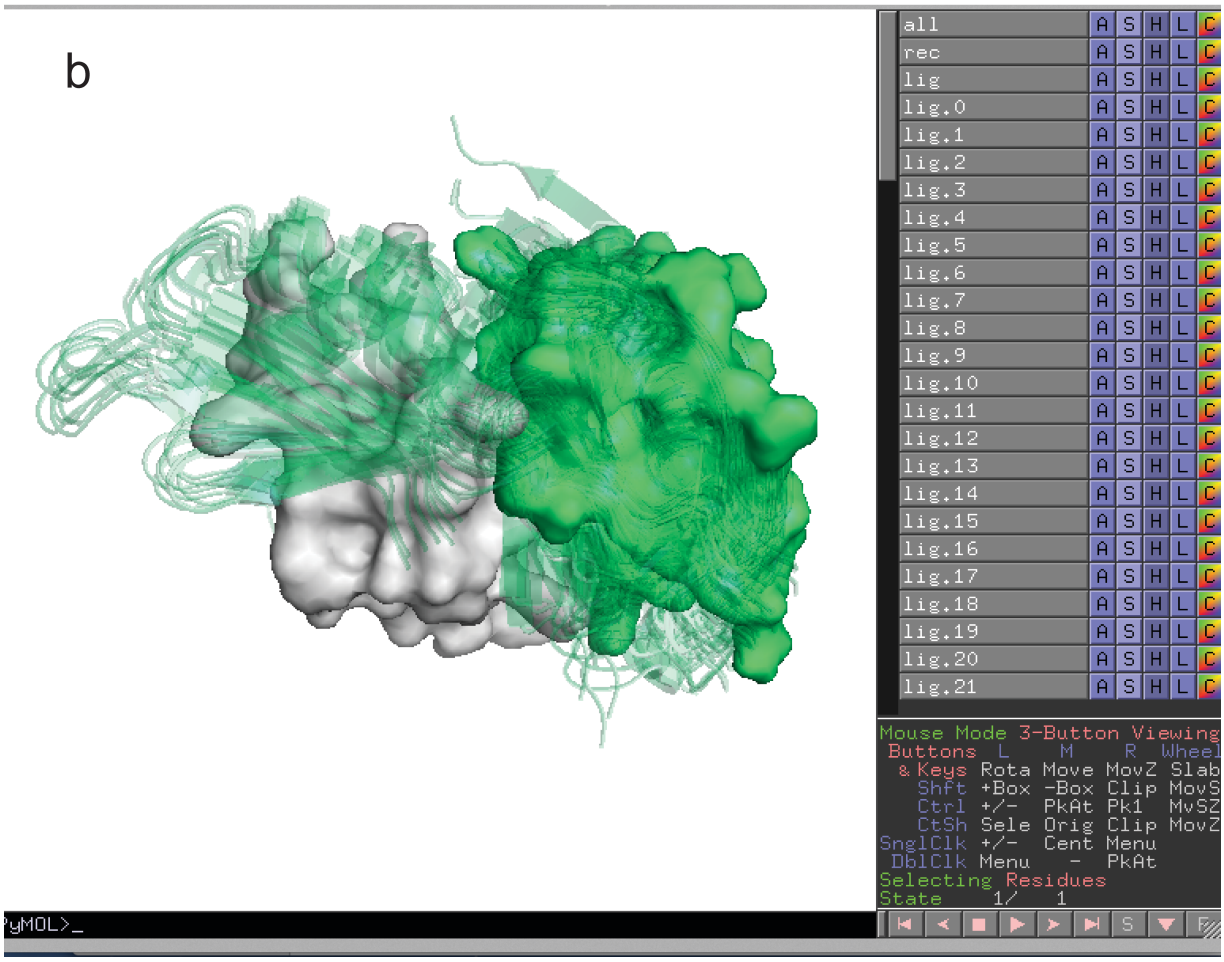



**Figure S3**

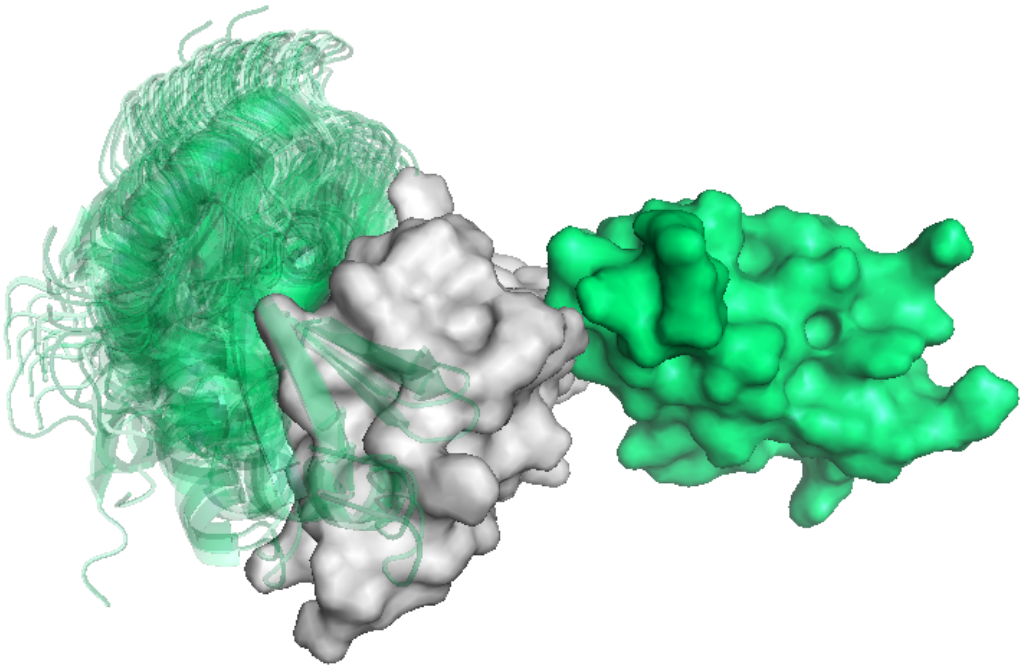


**Figure S4.** Results of the analysis of the interaction between chains A and C in CAPRI target T70 (Modulator protein MzrA, PDB ID 4pwu). The docked poses show strong interactions on the other side of subunit A. PyMOL generates a symmetry mate at that position, and the ClusPro result indicates a biological interface in addition to the one in the A:B dimer. This results in the stable A2:B2 tetramer (see text).

**Supplementary References**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[2] S. Dey, A. Pal, P. Chakrabarti, J. Janin, The subunit interfaces of weakly associated homodimeric proteins, J. Mol. Biol. 398 (2010) 146-60.

[3] R.P. Bahadur, P. Chakrabarti, F. Rodier, J. Janin, Dissecting subunit interfaces in homodimeric proteins, Proteins 53 (2003) 708-19.

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