Supplementary material: Table 1. Optimized direct pair potentials derived in the context of Rigid trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | −2.88 | ALA | ARG | 1.97 | ALA | ASN | 0.90 | ALA | ASP | 1.52 |
| ALA | CYS | −2.67 | ALA | GLN | 1.25 | ALA | GLU | 1.99 | ALA | GLY | 0.09 |
| ALA | HIS | −0.16 | ALA | ILE | −3.33 | ALA | LEU | −2.85 | ALA | LYS | 3.22 |
| ALA | MET | −0.56 | ALA | PHE | −1.30 | ALA | PRO | 1.17 | ALA | SER | −0.86 |
| ALA | THR | 0.34 | ALA | TRP | −1.34 | ALA | TYR | −1.55 | ALA | VAL | −3.15 |
| ARG | ARG | 2.31 | ARG | ASN | 1.63 | ARG | ASP | 1.80 | ARG | CYS | 0.75 |
| ARG | GLN | 2.14 | ARG | GLU | 1.66 | ARG | GLY | 0.77 | ARG | HIS | 0.41 |
| ARG | ILE | 1.45 | ARG | LEU | 1.96 | ARG | LYS | 3.48 | ARG | MET | 0.92 |
| ARG | PHE | 1.56 | ARG | PRO | 1.94 | ARG | SER | 1.70 | ARG | THR | 1.06 |
| ARG | TRP | −2.32 | ARG | TYR | 0.97 | ARG | VAL | 1.43 | ASN | ASN | −1.91 |
| ASN | ASP | 1.02 | ASN | CYS | 0.86 | ASN | GLN | 1.41 | ASN | GLU | 2.42 |
| ASN | GLY | 1.03 | ASN | HIS | 0.48 | ASN | ILE | 2.11 | ASN | LEU | 0.64 |
| ASN | LYS | 2.66 | ASN | MET | 1.69 | ASN | PHE | −0.45 | ASN | PRO | 0.09 |
| ASN | SER | 0.70 | ASN | THR | 1.14 | ASN | TRP | 1.48 | ASN | TYR | 0.97 |
| ASN | VAL | 2.68 | ASP | ASP | 1.73 | ASP | CYS | 1.46 | ASP | GLN | 2.99 |
| ASP | GLU | 3.13 | ASP | GLY | 1.41 | ASP | HIS | −0.35 | ASP | ILE | 1.77 |
| ASP | LEU | 2.67 | ASP | LYS | 2.49 | ASP | MET | 2.33 | ASP | PHE | 1.90 |
| ASP | PRO | 2.56 | ASP | SER | 0.63 | ASP | THR | 0.42 | ASP | TRP | 1.18 |
| ASP | TYR | 2.35 | ASP | VAL | 1.36 | CYS | CYS | −5.23 | CYS | GLN | 1.77 |
| CYS | GLU | −0.22 | CYS | GLY | −9.49 | CYS | HIS | −0.30 | CYS | ILE | −0.32 |
| CYS | LEU | −2.86 | CYS | LYS | 3.17 | CYS | MET | −0.64 | CYS | PHE | −2.10 |
| CYS | PRO | −1.74 | CYS | SER | −4.84 | CYS | THR | 0.42 | CYS | TRP | −1.08 |
| CYS | TYR | −2.07 | CYS | VAL | −2.63 | GLN | GLN | 0.08 | GLN | GLU | 2.65 |
| GLN | GLY | 1.13 | GLN | HIS | 1.76 | GLN | ILE | 1.50 | GLN | LEU | 1.42 |
| GLN | LYS | 2.67 | GLN | MET | −0.64 | GLN | PHE | −0.31 | GLN | PRO | 0.53 |
| GLN | SER | 1.83 | GLN | THR | 2.26 | GLN | TRP | 1.80 | GLN | TYR | 2.41 |
| GLN | VAL | 0.61 | GLU | GLU | 2.55 | GLU | GLY | 2.74 | GLU | HIS | 3.21 |
| GLU | ILE | 2.25 | GLU | LEU | 2.19 | GLU | LYS | 2.50 | GLU | MET | 1.39 |
| GLU | PHE | 1.87 | GLU | PRO | 1.99 | GLU | SER | 0.80 | GLU | THR | 1.72 |
| GLU | TRP | 3.17 | GLU | TYR | 1.63 | GLU | VAL | 2.80 | GLY | GLY | −3.77 |
| GLY | HIS | 0.95 | GLY | ILE | −2.84 | GLY | LEU | −0.42 | GLY | LYS | 2.37 |
| GLY | MET | −1.76 | GLY | PHE | 0.15 | GLY | PRO | 0.81 | GLY | SER | 0.11 |
| GLY | THR | −1.49 | GLY | TRP | −0.61 | GLY | TYR | −0.77 | GLY | VAL | −0.35 |
| HIS | HIS | −1.88 | HIS | ILE | 1.71 | HIS | LEU | −1.67 | HIS | LYS | 3.30 |
| HIS | MET | −1.06 | HIS | PHE | 0.65 | HIS | PRO | −0.36 | HIS | SER | 1.16 |
| HIS | THR | 2.09 | HIS | TRP | −0.44 | HIS | TYR | −1.41 | HIS | VAL | 0.12 |
| ILE | ILE | −8.67 | ILE | LEU | −3.70 | ILE | LYS | 3.52 | ILE | MET | −3.31 |
| ILE | PHE | −5.97 | ILE | PRO | −1.51 | ILE | SER | 1.05 | ILE | THR | −1.92 |
| ILE | TRP | −2.58 | ILE | TYR | −5.09 | ILE | VAL | −5.26 | LEU | LEU | −8.34 |
| LEU | LYS | 2.77 | LEU | MET | −1.92 | LEU | PHE | −4.86 | LEU | PRO | −0.31 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | −0.38 | LEU | THR | −0.24 | LEU | TRP | −2.85 | LEU | TYR | −0.27 |
| LEU | VAL | −5.07 | LYS | LYS | 2.54 | LYS | MET | 2.30 | LYS | PHE | 2.54 |
| LYS | PRO | 2.42 | LYS | SER | 2.37 | LYS | THR | 2.78 | LYS | TRP | 2.74 |
| LYS | TYR | 2.01 | LYS | VAL | 2.03 | MET | MET | −2.66 | MET | PHE | −3.23 |
| MET | PRO | 0.19 | MET | SER | −0.55 | MET | THR | 1.35 | MET | TRP | −0.42 |
| MET | TYR | −0.77 | MET | VAL | −3.69 | PHE | PHE | −5.09 | PHE | PRO | −2.35 |
| PHE | SER | 1.96 | PHE | THR | 0.36 | PHE | TRP | −1.96 | PHE | TYR | −1.30 |
| PHE | VAL | −4.74 | PRO | PRO | 1.49 | PRO | SER | 0.90 | PRO | THR | 0.91 |
| PRO | TRP | −3.27 | PRO | TYR | −2.29 | PRO | VAL | 0.02 | SER | SER | −0.80 |
| SER | THR | −0.17 | SER | TRP | −0.23 | SER | TYR | 1.25 | SER | VAL | 0.68 |
| THR | THR | −2.48 | THR | TRP | −4.71 | THR | TYR | 0.31 | THR | VAL | 0.20 |
| TRP | TRP | −0.61 | TRP | TYR | −1.63 | TRP | VAL | 0.93 | TYR | TYR | −3.47 |
| TYR | VAL | −1.54 | VAL | VAL | −13.07 | | | | | | |

Supplementary material: Table 2. Optimized water-mediated pair potentials derived in the context of Rigid trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | −0.22 | ALA | ARG | 1.00 | ALA | ASN | 0.20 | ALA | ASP | 0.66 |
| ALA | CYS | 0.54 | ALA | GLN | 0.83 | ALA | GLU | 1.11 | ALA | GLY | −2.03 |
| ALA | HIS | 1.59 | ALA | ILE | 0.45 | ALA | LEU | 0.32 | ALA | LYS | 0.02 |
| ALA | MET | 1.16 | ALA | PHE | −0.80 | ALA | PRO | −0.39 | ALA | SER | −1.03 |
| ALA | THR | −0.12 | ALA | TRP | 1.31 | ALA | TYR | 2.02 | ALA | VAL | −0.46 |
| ARG | ARG | −1.50 | ARG | ASN | −0.17 | ARG | ASP | −1.90 | ARG | CYS | 0.03 |
| ARG | GLN | −0.75 | ARG | GLU | −1.56 | ARG | GLY | −0.63 | ARG | HIS | −3.40 |
| ARG | ILE | −0.83 | ARG | LEU | 0.63 | ARG | LYS | 0.72 | ARG | MET | 0.94 |
| ARG | PHE | −0.73 | ARG | PRO | −0.05 | ARG | SER | −0.28 | ARG | THR | 0.21 |
| ARG | TRP | −0.34 | ARG | TYR | −2.54 | ARG | VAL | 1.16 | ASN | ASN | −2.55 |
| ASN | ASP | −1.14 | ASN | CYS | 1.15 | ASN | GLN | 0.90 | ASN | GLU | 0.73 |
| ASN | GLY | 0.04 | ASN | HIS | 1.42 | ASN | ILE | 2.50 | ASN | LEU | 0.31 |
| ASN | LYS | 1.75 | ASN | MET | −0.68 | ASN | PHE | 0.33 | ASN | PRO | −1.81 |
| ASN | SER | 0.52 | ASN | THR | 0.54 | ASN | TRP | −1.01 | ASN | TYR | 0.02 |
| ASN | VAL | 0.60 | ASP | ASP | −1.70 | ASP | CYS | 1.17 | ASP | GLN | 0.73 |
| ASP | GLU | 1.55 | ASP | GLY | 0.38 | ASP | HIS | −2.20 | ASP | ILE | 2.97 |
| ASP | LEU | 0.67 | ASP | LYS | −0.95 | ASP | MET | 1.06 | ASP | PHE | 2.31 |
| ASP | PRO | −0.21 | ASP | SER | −1.31 | ASP | THR | −1.47 | ASP | TRP | 1.25 |
| ASP | TYR | −1.37 | ASP | VAL | −0.14 | CYS | CYS | 0.40 | CYS | GLN | 1.15 |
| CYS | GLU | 0.21 | CYS | GLY | 0.60 | CYS | HIS | 0.42 | CYS | ILE | 0.93 |
| CYS | LEU | 0.92 | CYS | LYS | 1.88 | CYS | MET | 0.31 | CYS | PHE | 0.49 |
| CYS | PRO | 0.14 | CYS | SER | 0.36 | CYS | THR | 1.62 | CYS | TRP | 0.22 |
| CYS | TYR | 0.46 | CYS | VAL | 0.79 | GLN | GLN | 0.09 | GLN | GLU | 0.50 |
| GLN | GLY | −1.16 | GLN | HIS | 1.49 | GLN | ILE | 1.73 | GLN | LEU | −0.30 |
| GLN | LYS | 0.41 | GLN | MET | 0.47 | GLN | PHE | −1.08 | GLN | PRO | 0.01 |
| GLN | SER | 0.54 | GLN | THR | 0.50 | GLN | TRP | −0.70 | GLN | TYR | −0.85 |
| GLN | VAL | −0.71 | GLU | GLU | 0.77 | GLU | GLY | 0.12 | GLU | HIS | −2.05 |
| GLU | ILE | 1.65 | GLU | LEU | 1.72 | GLU | LYS | −1.07 | GLU | MET | 0.92 |
| GLU | PHE | 1.91 | GLU | PRO | 0.72 | GLU | SER | −0.06 | GLU | THR | 0.45 |
| GLU | TRP | 0.57 | GLU | TYR | −0.29 | GLU | VAL | 0.67 | GLY | GLY | −2.97 |
| GLY | HIS | −0.10 | GLY | ILE | 0.77 | GLY | LEU | 1.02 | GLY | LYS | 0.30 |
| GLY | MET | 0.27 | GLY | PHE | −2.72 | GLY | PRO | −0.31 | GLY | SER | 0.40 |
| GLY | THR | 0.99 | GLY | TRP | 0.52 | GLY | TYR | 0.50 | GLY | VAL | −1.17 |
| HIS | HIS | −0.73 | HIS | ILE | −1.10 | HIS | LEU | 0.10 | HIS | LYS | 1.52 |
| HIS | MET | 0.58 | HIS | PHE | −0.94 | HIS | PRO | −0.91 | HIS | SER | 0.95 |
| HIS | THR | −2.13 | HIS | TRP | −0.63 | HIS | TYR | −0.51 | HIS | VAL | 0.13 |
| ILE | ILE | −0.54 | ILE | LEU | −0.17 | ILE | LYS | 1.51 | ILE | MET | 0.81 |
| ILE | PHE | −1.72 | ILE | PRO | −0.85 | ILE | SER | 0.45 | ILE | THR | 1.20 |
| ILE | TRP | 0.14 | ILE | TYR | −1.37 | ILE | VAL | 0.18 | LEU | LEU | 0.49 |
| LEU | LYS | 0.73 | LEU | MET | −0.35 | LEU | PHE | −0.62 | LEU | PRO | 0.83 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | 0.48 | LEU | THR | 0.18 | LEU | TRP | 0.24 | LEU | TYR | −0.44 |
| LEU | VAL | 0.80 | LYS | LYS | 1.26 | LYS | MET | −0.69 | LYS | PHE | 0.22 |
| LYS | PRO | 0.37 | LYS | SER | 0.57 | LYS | THR | 0.30 | LYS | TRP | −1.32 |
| LYS | TYR | −0.85 | LYS | VAL | 1.58 | MET | MET | −0.79 | MET | PHE | 0.30 |
| MET | PRO | −0.26 | MET | SER | 1.67 | MET | THR | −0.29 | MET | TRP | 0.40 |
| MET | TYR | −1.35 | MET | VAL | −1.81 | PHE | PHE | −1.47 | PHE | PRO | 0.31 |
| PHE | SER | 0.79 | PHE | THR | 1.95 | PHE | TRP | 0.15 | PHE | TYR | −0.58 |
| PHE | VAL | −1.08 | PRO | PRO | −0.36 | PRO | SER | 0.76 | PRO | THR | −0.06 |
| PRO | TRP | −2.20 | PRO | TYR | −3.50 | PRO | VAL | 0.46 | SER | SER | −1.19 |
| SER | THR | −0.50 | SER | TRP | 0.60 | SER | TYR | −2.29 | SER | VAL | 0.97 |
| THR | THR | −3.10 | THR | TRP | −1.64 | THR | TYR | 0.16 | THR | VAL | 0.67 |
| TRP | TRP | −0.98 | TRP | TYR | −1.62 | TRP | VAL | 0.82 | TYR | TYR | −1.91 |
| TYR | VAL | 0.73 | VAL | VAL | −0.58 | | | | | | |

Supplementary material: Table 3. Optimized direct pair potentials derived in the context of Semi-Flexible trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | −3.18 | ALA | ARG | 2.24 | ALA | ASN | 0.98 | ALA | ASP | 1.68 |
| ALA | CYS | −3.88 | ALA | GLN | 1.14 | ALA | GLU | 1.64 | ALA | GLY | 0.67 |
| ALA | HIS | 0.02 | ALA | ILE | −3.11 | ALA | LEU | −2.35 | ALA | LYS | 3.21 |
| ALA | MET | −0.21 | ALA | PHE | −0.87 | ALA | PRO | 1.23 | ALA | SER | −0.86 |
| ALA | THR | 0.54 | ALA | TRP | −0.72 | ALA | TYR | −0.79 | ALA | VAL | −3.09 |
| ARG | ARG | 2.06 | ARG | ASN | 1.45 | ARG | ASP | 1.58 | ARG | CYS | 1.10 |
| ARG | GLN | 2.07 | ARG | GLU | 1.09 | ARG | GLY | 1.00 | ARG | HIS | 0.49 |
| ARG | ILE | 1.84 | ARG | LEU | 2.32 | ARG | LYS | 3.65 | ARG | MET | 0.78 |
| ARG | PHE | 1.69 | ARG | PRO | 1.97 | ARG | SER | 1.91 | ARG | THR | 1.26 |
| ARG | TRP | −3.05 | ARG | TYR | 1.34 | ARG | VAL | 1.81 | ASN | ASN | −3.03 |
| ASN | ASP | 0.77 | ASN | CYS | 1.21 | ASN | GLN | 1.27 | ASN | GLU | 2.36 |
| ASN | GLY | 1.27 | ASN | HIS | 0.33 | ASN | ILE | 2.70 | ASN | LEU | 0.83 |
| ASN | LYS | 2.47 | ASN | MET | 2.01 | ASN | PHE | −0.43 | ASN | PRO | −0.22 |
| ASN | SER | 0.60 | ASN | THR | 1.12 | ASN | TRP | 2.55 | ASN | TYR | 1.46 |
| ASN | VAL | 3.35 | ASP | ASP | 1.40 | ASP | CYS | 2.28 | ASP | GLN | 3.04 |
| ASP | GLU | 3.07 | ASP | GLY | 1.73 | ASP | HIS | −0.78 | ASP | ILE | 2.26 |
| ASP | LEU | 3.44 | ASP | LYS | 2.14 | ASP | MET | 2.76 | ASP | PHE | 2.36 |
| ASP | PRO | 2.79 | ASP | SER | 0.61 | ASP | THR | 0.46 | ASP | TRP | 2.20 |
| ASP | TYR | 2.70 | ASP | VAL | 1.80 | CYS | CYS | −4.72 | CYS | GLN | 2.26 |
| CYS | GLU | −0.51 | CYS | GLY | −4.72 | CYS | HIS | −0.21 | CYS | ILE | −0.31 |
| CYS | LEU | −3.24 | CYS | LYS | 3.73 | CYS | MET | −1.03 | CYS | PHE | −2.62 |
| CYS | PRO | −2.72 | CYS | SER | −4.72 | CYS | THR | 0.65 | CYS | TRP | −1.40 |
| CYS | TYR | −2.36 | CYS | VAL | −3.09 | GLN | GLN | −0.84 | GLN | GLU | 2.50 |
| GLN | GLY | 1.25 | GLN | HIS | 2.18 | GLN | ILE | 1.92 | GLN | LEU | 1.67 |
| GLN | LYS | 2.56 | GLN | MET | −1.30 | GLN | PHE | −0.83 | GLN | PRO | 0.14 |
| GLN | SER | 1.92 | GLN | THR | 2.46 | GLN | TRP | 2.72 | GLN | TYR | 2.82 |
| GLN | VAL | 0.72 | GLU | GLU | 2.08 | GLU | GLY | 2.86 | GLU | HIS | 3.46 |
| GLU | ILE | 2.34 | GLU | LEU | 2.30 | GLU | LYS | 2.05 | GLU | MET | 0.87 |
| GLU | PHE | 1.63 | GLU | PRO | 1.59 | GLU | SER | 0.52 | GLU | THR | 1.49 |
| GLU | TRP | 3.79 | GLU | TYR | 1.55 | GLU | VAL | 3.04 | GLY | GLY | −3.70 |
| GLY | HIS | 1.47 | GLY | ILE | −1.83 | GLY | LEU | 0.20 | GLY | LYS | 2.05 |
| GLY | MET | −1.20 | GLY | PHE | 1.02 | GLY | PRO | 1.03 | GLY | SER | 0.32 |
| GLY | THR | −1.04 | GLY | TRP | −0.08 | GLY | TYR | 0.33 | GLY | VAL | 0.44 |
| HIS | HIS | −2.85 | HIS | ILE | 3.06 | HIS | LEU | −2.37 | HIS | LYS | 3.49 |
| HIS | MET | −1.65 | HIS | PHE | 1.02 | HIS | PRO | −0.82 | HIS | SER | 1.59 |
| HIS | THR | 2.51 | HIS | TRP | −0.52 | HIS | TYR | −1.37 | HIS | VAL | 0.20 |
| ILE | ILE | −4.72 | ILE | LEU | −3.28 | ILE | LYS | 3.72 | ILE | MET | −3.75 |
| ILE | PHE | −4.72 | ILE | PRO | −1.78 | ILE | SER | 1.90 | ILE | THR | −1.65 |
| ILE | TRP | −2.85 | ILE | TYR | −3.25 | ILE | VAL | −4.72 | LEU | LEU | −4.72 |
| LEU | LYS | 2.79 | LEU | MET | −2.10 | LEU | PHE | −4.72 | LEU | PRO | −0.30 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | 0.10 | LEU | THR | 0.26 | LEU | TRP | −3.23 | LEU | TYR | 0.80 |
| LEU | VAL | −4.72 | LYS | LYS | 2.08 | LYS | MET | 2.00 | LYS | PHE | 2.47 |
| LYS | PRO | 2.24 | LYS | SER | 2.26 | LYS | THR | 2.70 | LYS | TRP | 2.87 |
| LYS | TYR | 1.84 | LYS | VAL | 1.96 | MET | MET | −3.78 | MET | PHE | −4.63 |
| MET | PRO | −0.11 | MET | SER | −0.80 | MET | THR | 1.81 | MET | TRP | −0.36 |
| MET | TYR | −0.29 | MET | VAL | −4.72 | PHE | PHE | −4.72 | PHE | PRO | −3.24 |
| PHE | SER | 2.79 | PHE | THR | 0.59 | PHE | TRP | −2.39 | PHE | TYR | −0.13 |
| PHE | VAL | −4.72 | PRO | PRO | 1.33 | PRO | SER | 0.95 | PRO | THR | 0.88 |
| PRO | TRP | −4.32 | PRO | TYR | −1.86 | PRO | VAL | −0.02 | SER | SER | −1.53 |
| SER | THR | 0.01 | SER | TRP | 0.57 | SER | TYR | 1.88 | SER | VAL | 1.15 |
| THR | THR | −2.66 | THR | TRP | −4.54 | THR | TYR | 1.14 | THR | VAL | 0.94 |
| TRP | TRP | −0.75 | TRP | TYR | −1.64 | TRP | VAL | 1.56 | TYR | TYR | −3.68 |
| TYR | VAL | −0.46 | VAL | VAL | −4.72 | | | | | | |

Supplementary material: Table 4. Optimized water-mediated pair potentials derived in the context of Semi-Flexible trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | 0.53 | ALA | ARG | 1.19 | ALA | ASN | 0.12 | ALA | ASP | 0.75 |
| ALA | CYS | 0.90 | ALA | GLN | 0.71 | ALA | GLU | 0.78 | ALA | GLY | −1.52 |
| ALA | HIS | 2.32 | ALA | ILE | 1.20 | ALA | LEU | 0.90 | ALA | LYS | −1.02 |
| ALA | MET | 2.04 | ALA | PHE | −0.31 | ALA | PRO | −0.59 | ALA | SER | −0.85 |
| ALA | THR | 0.14 | ALA | TRP | 2.37 | ALA | TYR | 2.85 | ALA | VAL | 0.21 |
| ARG | ARG | −3.33 | ARG | ASN | −0.83 | ARG | ASP | −2.99 | ARG | CYS | 0.17 |
| ARG | GLN | −1.80 | ARG | GLU | −3.66 | ARG | GLY | −0.63 | ARG | HIS | −4.72 |
| ARG | ILE | −0.93 | ARG | LEU | 0.87 | ARG | LYS | −0.41 | ARG | MET | 1.00 |
| ARG | PHE | −1.07 | ARG | PRO | −0.60 | ARG | SER | −0.39 | ARG | THR | 0.23 |
| ARG | TRP | −0.37 | ARG | TYR | −2.42 | ARG | VAL | 1.51 | ASN | ASN | −3.84 |
| ASN | ASP | −1.74 | ASN | CYS | 1.87 | ASN | GLN | 0.58 | ASN | GLU | 0.07 |
| ASN | GLY | 0.26 | ASN | HIS | 1.84 | ASN | ILE | 3.06 | ASN | LEU | 0.53 |
| ASN | LYS | 1.31 | ASN | MET | −1.04 | ASN | PHE | 0.72 | ASN | PRO | −2.92 |
| ASN | SER | 0.49 | ASN | THR | 0.47 | ASN | TRP | −1.10 | ASN | TYR | 0.43 |
| ASN | VAL | 0.95 | ASP | ASP | −3.00 | ASP | CYS | 1.85 | ASP | GLN | 0.25 |
| ASP | GLU | 0.99 | ASP | GLY | 0.61 | ASP | HIS | −3.00 | ASP | ILE | 3.58 |
| ASP | LEU | 1.13 | ASP | LYS | −2.66 | ASP | MET | 1.43 | ASP | PHE | 2.91 |
| ASP | PRO | −0.75 | ASP | SER | −1.62 | ASP | THR | −1.49 | ASP | TRP | 2.09 |
| ASP | TYR | −1.01 | ASP | VAL | 0.09 | CYS | CYS | 0.70 | CYS | GLN | 1.63 |
| CYS | GLU | 0.38 | CYS | GLY | 1.25 | CYS | HIS | 0.77 | CYS | ILE | 1.46 |
| CYS | LEU | 1.73 | CYS | LYS | 2.55 | CYS | MET | 0.47 | CYS | PHE | 0.91 |
| CYS | PRO | 0.32 | CYS | SER | 0.90 | CYS | THR | 2.52 | CYS | TRP | 0.43 |
| CYS | TYR | 1.01 | CYS | VAL | 1.67 | GLN | GLN | −0.85 | GLN | GLU | −0.25 |
| GLN | GLY | −1.54 | GLN | HIS | 1.87 | GLN | ILE | 2.17 | GLN | LEU | −0.37 |
| GLN | LYS | −0.63 | GLN | MET | 0.43 | GLN | PHE | −1.66 | GLN | PRO | −0.61 |
| GLN | SER | 0.24 | GLN | THR | 0.48 | GLN | TRP | −0.76 | GLN | TYR | −0.79 |
| GLN | VAL | −0.86 | GLU | GLU | −0.86 | GLU | GLY | −0.19 | GLU | HIS | −3.94 |
| GLU | ILE | 1.89 | GLU | LEU | 1.83 | GLU | LYS | −3.92 | GLU | MET | 0.38 |
| GLU | PHE | 1.99 | GLU | PRO | −0.22 | GLU | SER | −0.49 | GLU | THR | −0.00 |
| GLU | TRP | 0.68 | GLU | TYR | −0.38 | GLU | VAL | 0.57 | GLY | GLY | −2.61 |
| GLY | HIS | 0.27 | GLY | ILE | 1.71 | GLY | LEU | 1.83 | GLY | LYS | −0.32 |
| GLY | MET | 1.12 | GLY | PHE | −2.22 | GLY | PRO | −0.33 | GLY | SER | 0.77 |
| GLY | THR | 1.77 | GLY | TRP | 1.30 | GLY | TYR | 1.34 | GLY | VAL | −0.30 |
| HIS | HIS | −1.13 | HIS | ILE | −1.16 | HIS | LEU | 0.12 | HIS | LYS | 1.12 |
| HIS | MET | 0.70 | HIS | PHE | −1.27 | HIS | PRO | −1.56 | HIS | SER | 1.39 |
| HIS | THR | −2.80 | HIS | TRP | −0.84 | HIS | TYR | −0.35 | HIS | VAL | 0.38 |
| ILE | ILE | −0.29 | ILE | LEU | 0.39 | ILE | LYS | 1.38 | ILE | MET | 1.43 |
| ILE | PHE | −1.81 | ILE | PRO | −0.77 | ILE | SER | 1.14 | ILE | THR | 1.86 |
| ILE | TRP | 0.50 | ILE | TYR | −0.87 | ILE | VAL | 1.10 | LEU | LEU | 0.71 |
| LEU | LYS | 0.40 | LEU | MET | −0.17 | LEU | PHE | −0.37 | LEU | PRO | 1.13 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | 1.05 | LEU | THR | 0.59 | LEU | TRP | 0.71 | LEU | TYR | 0.17 |
| LEU | VAL | 1.62 | LYS | LYS | −0.41 | LYS | MET | −2.02 | LYS | PHE | −0.30 |
| LYS | PRO | −0.79 | LYS | SER | −0.08 | LYS | THR | −0.52 | LYS | TRP | −2.13 |
| LYS | TYR | −1.47 | LYS | VAL | 1.61 | MET | MET | −1.10 | MET | PHE | 0.42 |
| MET | PRO | −0.44 | MET | SER | 2.54 | MET | THR | −0.30 | MET | TRP | 0.62 |
| MET | TYR | −1.50 | MET | VAL | −2.29 | PHE | PHE | −1.96 | PHE | PRO | 0.59 |
| PHE | SER | 1.48 | PHE | THR | 2.73 | PHE | TRP | 0.40 | PHE | TYR | −0.03 |
| PHE | VAL | −0.74 | PRO | PRO | −1.51 | PRO | SER | 0.82 | PRO | THR | −0.18 |
| PRO | TRP | −2.92 | PRO | TYR | −3.29 | PRO | VAL | 0.80 | SER | SER | −1.84 |
| SER | THR | −0.12 | SER | TRP | 1.25 | SER | TYR | −1.83 | SER | VAL | 1.59 |
| THR | THR | −3.22 | THR | TRP | −1.56 | THR | TYR | 0.90 | THR | VAL | 1.39 |
| TRP | TRP | −1.30 | TRP | TYR | −1.93 | TRP | VAL | 1.37 | TYR | TYR | −2.02 |
| TYR | VAL | 1.91 | VAL | VAL | −0.02 | | | | | | |

Supplementary material: Table 5. Optimized direct pair potentials derived in the context of Flexible trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | −2.11 | ALA | ARG | 1.60 | ALA | ASN | 0.36 | ALA | ASP | 0.88 |
| ALA | CYS | −0.89 | ALA | GLN | 0.12 | ALA | GLU | 0.60 | ALA | GLY | 0.73 |
| ALA | HIS | −0.14 | ALA | ILE | −0.41 | ALA | LEU | −0.36 | ALA | LYS | 2.23 |
| ALA | MET | 0.72 | ALA | PHE | 0.43 | ALA | PRO | 0.89 | ALA | SER | −0.95 |
| ALA | THR | 0.38 | ALA | TRP | 0.20 | ALA | TYR | −0.19 | ALA | VAL | −0.71 |
| ARG | ARG | 0.87 | ARG | ASN | 0.02 | ARG | ASP | 0.08 | ARG | CYS | 1.74 |
| ARG | GLN | 0.97 | ARG | GLU | −1.01 | ARG | GLY | −0.27 | ARG | HIS | −1.90 |
| ARG | ILE | 1.20 | ARG | LEU | 1.62 | ARG | LYS | 4.14 | ARG | MET | −0.39 |
| ARG | PHE | 1.09 | ARG | PRO | 0.49 | ARG | SER | 1.00 | ARG | THR | −0.09 |
| ARG | TRP | −3.69 | ARG | TYR | 0.29 | ARG | VAL | 1.20 | ASN | ASN | −4.47 |
| ASN | ASP | −0.94 | ASN | CYS | 1.83 | ASN | GLN | −0.19 | ASN | GLU | 1.36 |
| ASN | GLY | 0.45 | ASN | HIS | −1.10 | ASN | ILE | 2.21 | ASN | LEU | 0.64 |
| ASN | LYS | 1.64 | ASN | MET | 1.56 | ASN | PHE | −0.66 | ASN | PRO | −2.37 |
| ASN | SER | −0.83 | ASN | THR | 0.09 | ASN | TRP | 2.13 | ASN | TYR | 0.67 |
| ASN | VAL | 2.71 | ASP | ASP | −0.20 | ASP | CYS | 2.63 | ASP | GLN | 2.62 |
| ASP | GLU | 2.71 | ASP | GLY | 0.72 | ASP | HIS | −3.07 | ASP | ILE | 1.56 |
| ASP | LEU | 2.61 | ASP | LYS | 1.20 | ASP | MET | 2.05 | ASP | PHE | 1.65 |
| ASP | PRO | 2.10 | ASP | SER | −0.76 | ASP | THR | −1.02 | ASP | TRP | 1.42 |
| ASP | TYR | 2.04 | ASP | VAL | 1.09 | CYS | CYS | −4.47 | CYS | GLN | 2.73 |
| CYS | GLU | 0.09 | CYS | GLY | −4.47 | CYS | HIS | 0.60 | CYS | ILE | 1.60 |
| CYS | LEU | −0.35 | CYS | LYS | 2.92 | CYS | MET | 0.10 | CYS | PHE | −0.87 |
| CYS | PRO | −1.45 | CYS | SER | −4.06 | CYS | THR | 1.49 | CYS | TRP | −0.73 |
| CYS | TYR | −0.99 | CYS | VAL | −0.11 | GLN | GLN | −3.44 | GLN | GLU | 1.75 |
| GLN | GLY | 0.28 | GLN | HIS | 1.02 | GLN | ILE | 1.29 | GLN | LEU | 1.10 |
| GLN | LYS | 2.04 | GLN | MET | −2.23 | GLN | PHE | −1.28 | GLN | PRO | −1.79 |
| GLN | SER | 1.02 | GLN | THR | 1.78 | GLN | TRP | 2.43 | GLN | TYR | 2.30 |
| GLN | VAL | 0.20 | GLU | GLU | 0.92 | GLU | GLY | 2.02 | GLU | HIS | 2.79 |
| GLU | ILE | 1.48 | GLU | LEU | 1.46 | GLU | LYS | 1.11 | GLU | MET | −0.14 |
| GLU | PHE | 0.77 | GLU | PRO | −0.10 | GLU | SER | −1.37 | GLU | THR | 0.14 |
| GLU | TRP | 3.17 | GLU | TYR | 0.34 | GLU | VAL | 2.07 | GLY | GLY | −3.87 |
| GLY | HIS | 0.84 | GLY | ILE | −0.43 | GLY | LEU | 0.90 | GLY | LYS | 0.71 |
| GLY | MET | −0.84 | GLY | PHE | 1.41 | GLY | PRO | 0.29 | GLY | SER | −0.33 |
| GLY | THR | −1.83 | GLY | TRP | 0.08 | GLY | TYR | 0.11 | GLY | VAL | 1.08 |
| HIS | HIS | −3.36 | HIS | ILE | 2.67 | HIS | LEU | −1.56 | HIS | LYS | 2.93 |
| HIS | MET | −1.65 | HIS | PHE | 1.39 | HIS | PRO | −2.80 | HIS | SER | 0.95 |
| HIS | THR | 1.89 | HIS | TRP | −0.39 | HIS | TYR | −1.75 | HIS | VAL | 0.60 |
| ILE | ILE | −3.90 | ILE | LEU | −0.25 | ILE | LYS | 2.51 | ILE | MET | −1.20 |
| ILE | PHE | −1.82 | ILE | PRO | −1.00 | ILE | SER | 1.89 | ILE | THR | −0.69 |
| ILE | TRP | −1.83 | ILE | TYR | −1.27 | ILE | VAL | −0.83 | LEU | LEU | −4.38 |
| LEU | LYS | 1.68 | LEU | MET | −0.24 | LEU | PHE | −1.20 | LEU | PRO | 0.01 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | 0.52 | LEU | THR | 0.63 | LEU | TRP | −0.97 | LEU | TYR | 1.44 |
| LEU | VAL | −0.98 | LYS | LYS | 1.23 | LYS | MET | 0.85 | LYS | PHE | 1.26 |
| LYS | PRO | 0.92 | LYS | SER | 1.21 | LYS | THR | 2.03 | LYS | TRP | 1.85 |
| LYS | TYR | 0.42 | LYS | VAL | 0.68 | MET | MET | −3.51 | MET | PHE | −3.08 |
| MET | PRO | −0.40 | MET | SER | −0.36 | MET | THR | 1.66 | MET | TRP | 0.11 |
| MET | TYR | 0.30 | MET | VAL | −1.49 | PHE | PHE | −4.47 | PHE | PRO | −2.79 |
| PHE | SER | 2.51 | PHE | THR | 0.74 | PHE | TRP | −1.23 | PHE | TYR | 0.76 |
| PHE | VAL | −1.33 | PRO | PRO | −0.02 | PRO | SER | −0.18 | PRO | THR | −0.23 |
| PRO | TRP | −4.15 | PRO | TYR | −2.85 | PRO | VAL | 0.19 | SER | SER | −3.49 |
| SER | THR | −1.27 | SER | TRP | 0.58 | SER | TYR | 1.41 | SER | VAL | 1.33 |
| THR | THR | −4.33 | THR | TRP | −4.01 | THR | TYR | 0.60 | THR | VAL | 0.90 |
| TRP | TRP | −0.49 | TRP | TYR | −1.06 | TRP | VAL | 2.16 | TYR | TYR | −3.58 |
| TYR | VAL | 0.26 | VAL | VAL | −4.47 | | | | | | |

Supplementary material: Table 6. Optimized water-mediated pair potentials derived in the context of Flexible trap states.

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ALA | ALA | 0.94 | ALA | ARG | 1.58 | ALA | ASN | 0.44 | ALA | ASP | 1.10 |
| ALA | CYS | 2.55 | ALA | GLN | 0.94 | ALA | GLU | 0.93 | ALA | GLY | −0.40 |
| ALA | HIS | 2.78 | ALA | ILE | 1.97 | ALA | LEU | 1.74 | ALA | LYS | −1.25 |
| ALA | MET | 2.89 | ALA | PHE | 1.17 | ALA | PRO | 0.04 | ALA | SER | −0.20 |
| ALA | THR | 0.74 | ALA | TRP | 3.39 | ALA | TYR | 3.20 | ALA | VAL | 1.45 |
| ARG | ARG | −4.47 | ARG | ASN | −2.88 | ARG | ASP | −4.47 | ARG | CYS | 1.15 |
| ARG | GLN | −4.47 | ARG | GLU | −4.47 | ARG | GLY | −1.27 | ARG | HIS | −4.47 |
| ARG | ILE | 0.17 | ARG | LEU | 1.54 | ARG | LYS | −3.19 | ARG | MET | 0.85 |
| ARG | PHE | −0.38 | ARG | PRO | −2.67 | ARG | SER | −1.54 | ARG | THR | −0.38 |
| ARG | TRP | −0.33 | ARG | TYR | −3.36 | ARG | VAL | 2.24 | ASN | ASN | −4.47 |
| ASN | ASP | −3.95 | ASN | CYS | 2.76 | ASN | GLN | −0.42 | ASN | GLU | −1.35 |
| ASN | GLY | 0.07 | ASN | HIS | 0.95 | ASN | ILE | 3.39 | ASN | LEU | 1.20 |
| ASN | LYS | 0.52 | ASN | MET | −0.69 | ASN | PHE | 1.28 | ASN | PRO | −4.47 |
| ASN | SER | −0.17 | ASN | THR | 0.05 | ASN | TRP | −0.80 | ASN | TYR | 0.25 |
| ASN | VAL | 1.52 | ASP | ASP | −4.47 | ASP | CYS | 2.93 | ASP | GLN | −0.94 |
| ASP | GLU | −0.17 | ASP | GLY | 0.51 | ASP | HIS | −4.47 | ASP | ILE | 3.97 |
| ASP | LEU | 1.74 | ASP | LYS | −4.47 | ASP | MET | 1.44 | ASP | PHE | 3.41 |
| ASP | PRO | −2.44 | ASP | SER | −3.03 | ASP | THR | −2.66 | ASP | TRP | 2.25 |
| ASP | TYR | −1.42 | ASP | VAL | 0.73 | CYS | CYS | 1.32 | CYS | GLN | 2.34 |
| CYS | GLU | 1.71 | CYS | GLY | 2.96 | CYS | HIS | 1.32 | CYS | ILE | 2.71 |
| CYS | LEU | 3.17 | CYS | LYS | 3.65 | CYS | MET | 1.12 | CYS | PHE | 1.96 |
| CYS | PRO | 1.49 | CYS | SER | 2.28 | CYS | THR | 3.86 | CYS | TRP | 0.86 |
| CYS | TYR | 1.98 | CYS | VAL | 3.15 | GLN | GLN | −1.67 | GLN | GLU | −2.21 |
| GLN | GLY | −2.06 | GLN | HIS | 1.07 | GLN | ILE | 2.76 | GLN | LEU | 0.41 |
| GLN | LYS | −2.99 | GLN | MET | 0.53 | GLN | PHE | −1.14 | GLN | PRO | −1.94 |
| GLN | SER | −0.36 | GLN | THR | 0.14 | GLN | TRP | −0.52 | GLN | TYR | −0.85 |
| GLN | VAL | −0.14 | GLU | GLU | −3.85 | GLU | GLY | −0.89 | GLU | HIS | −4.47 |
| GLU | ILE | 2.44 | GLU | LEU | 2.36 | GLU | LYS | −4.47 | GLU | MET | 0.44 |
| GLU | PHE | 2.50 | GLU | PRO | −1.96 | GLU | SER | −1.67 | GLU | THR | −0.80 |
| GLU | TRP | 0.72 | GLU | TYR | −1.01 | GLU | VAL | 1.02 | GLY | GLY | −2.02 |
| GLY | HIS | 0.23 | GLY | ILE | 2.44 | GLY | LEU | 2.41 | GLY | LYS | −1.32 |
| GLY | MET | 1.85 | GLY | PHE | −0.34 | GLY | PRO | −0.37 | GLY | SER | 0.95 |
| GLY | THR | 2.04 | GLY | TRP | 2.14 | GLY | TYR | 1.82 | GLY | VAL | 1.13 |
| HIS | HIS | −1.36 | HIS | ILE | −0.36 | HIS | LEU | 1.00 | HIS | LYS | −0.17 |
| HIS | MET | 0.84 | HIS | PHE | −0.67 | HIS | PRO | −2.30 | HIS | SER | 1.07 |
| HIS | THR | −3.23 | HIS | TRP | −0.58 | HIS | TYR | −0.40 | HIS | VAL | 1.14 |
| ILE | ILE | 0.79 | ILE | LEU | 1.38 | ILE | LYS | 2.08 | ILE | MET | 2.56 |
| ILE | PHE | 0.01 | ILE | PRO | 0.73 | ILE | SER | 2.10 | ILE | THR | 2.49 |
| ILE | TRP | 1.30 | ILE | TYR | 0.63 | ILE | VAL | 1.91 | LEU | LEU | 1.45 |
| LEU | LYS | 0.83 | LEU | MET | 1.15 | LEU | PHE | 1.42 | LEU | PRO | 2.01 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| LEU | SER | 1.82 | LEU | THR | 1.47 | LEU | TRP | 1.93 | LEU | TYR | 1.51 |
| LEU | VAL | 2.11 | LYS | LYS | −3.38 | LYS | MET | −2.10 | LYS | PHE | −0.04 |
| LYS | PRO | −3.24 | LYS | SER | −1.44 | LYS | THR | −1.77 | LYS | TRP | −2.11 |
| LYS | TYR | −2.89 | LYS | VAL | 1.92 | MET | MET | −0.82 | MET | PHE | 1.34 |
| MET | PRO | −0.01 | MET | SER | 3.26 | MET | THR | 0.42 | MET | TRP | 0.96 |
| MET | TYR | −0.78 | MET | VAL | −0.72 | PHE | PHE | −0.97 | PHE | PRO | 1.50 |
| PHE | SER | 2.17 | PHE | THR | 3.15 | PHE | TRP | 1.15 | PHE | TYR | 1.11 |
| PHE | VAL | 1.02 | PRO | PRO | −2.71 | PRO | SER | 0.61 | PRO | THR | −0.73 |
| PRO | TRP | −2.42 | PRO | TYR | −3.44 | PRO | VAL | 1.65 | SER | SER | −3.19 |
| SER | THR | −0.61 | SER | TRP | 1.79 | SER | TYR | −1.94 | SER | VAL | 2.21 |
| THR | THR | −3.96 | THR | TRP | −0.90 | THR | TYR | 1.24 | THR | VAL | 1.99 |
| TRP | TRP | −1.03 | TRP | TYR | −1.29 | TRP | VAL | 2.44 | TYR | TYR | −1.71 |
| TYR | VAL | 2.41 | VAL | VAL | 1.18 | | | | | | |

Supplementary material: Table 7. PDB identifiers and chain names for the training set of protein complexes.

| | | | | | |
|---|---|---|---|---|---|
| 1AAR-A-B | 1AKS-A-B | 1AOR-A-B | 1APY-A-C | 1BBP-B-D | 1BCM-A-B |
| 1BHM-A-B | 1BMF-C-D | 1BND-A-B | 1BSR-A-B | 1CDC-A-B | 1CHO-E-I |
| 1CPC-A-B | 1CYD-C-D | 1DER-F-G | 1DOK-A-B | 1DVR-A-B | 1ECM-A-B |
| 1EPT-A-C | 1FAG-A-C | 1FC1-A-B | 1FLE-E-I | 1FUQ-A-B | 1GFL-A-B |
| 1GLU-A-B | 1GRI-A-B | 1GTP-B-I | 1HCG-A-B | 1HIW-A-R | 1HLP-A-B |
| 1HSB-A-B | 1KNY-A-B | 1LEH-A-B | 1LTS-A-C | 1LWI-A-B | 1MAS-A-B |
| 1MDY-A-B | 1MHL-A-C | 1MSA-A-D | 1NAL-2-3 | 1NCI-A-B | 1NOY-A-B |
| 1OBP-A-B | 1ONE-A-B | 1ORT-B-F | 1OTG-B-C | 1OVO-A-B | 1PIO-A-B |
| 1PNK-A-B | 1PRT-A-F | 1PSA-A-B | 1PVC-1-3 | 1PVU-A-B | 1PYT-A-C |
| 1QRD-A-B | 1RCO-R-V | 1RTH-A-B | 1RVV-1-2 | 1SCU-D-E | 1SFT-A-B |
| 1SRI-A-B | 1SVA-2-3 | 1TBR-K-S | 1THE-A-B | 1TII-E-F | 1TME-1-3 |
| 1TRK-A-B | 1TTA-A-B | 1UCY-E-H | 1VFB-A-B | 1VRT-A-B | 1WDC-A-C |
| 1WTL-A-B | 1XSO-A-B | 1YPT-A-B | 2BBK-H-L | 2BTF-A-P | 2CST-A-B |
| 2GLS-B-H | 2KAI-B-I | 2LIG-A-B | 2MEV-1-2 | 2PHL-B-C | 2POL-A-B |
| 2RSP-A-B | 2ZTA-A-B | 3PGA-2-4 | 4AAH-C-D | 4HTC-H-I | 4SGB-E-I |
| 6GSV-A-B | 8CAT-A-B | 1ABR-A-B | 1ADU-A-B | 1APX-A-B | 1ASY-A-B |
| 1BBB-A-B | 1BDM-A-B | 1BIN-A-B | 1BMV-1-2 | 1BPL-A-B | 1BVP-2-3 |
| 1CGJ-E-I | 1CHR-A-B | 1CPC-A-K | 1DAA-A-B | 1DIF-A-B | 1ECE-A-B |
| 1EPT-B-C | 1FAT-A-B | 1FIE-A-B | 1FVP-A-B | 1GDT-A-B | 1GIF-B-C |
| 1GYL-A-B | 1HJR-B-D | 1HMP-A-B | 1HTM-D-F | 1HUC-A-B | 1HYH-A-B |
| 1IDS-A-C | 1INH-A-B | 1KPB-A-B | 1LTS-D-E | 1MCO-H-L | 1MEC-1-4 |
| 1NHK-L-R | 1ORD-A-B | 1OSJ-A-B | 1OVA-A-B | 1PDG-A-B | 1PP2-L-R |
| 1PRT-H-J | 1PSD-A-B | 1PVC-3-4 | 1PXT-A-B | 1RCP-A-B | 1RTM-1-2 |
| 1SCE-B-D | 1SGP-E-I | 1STF-E-I | 1TAB-E-I | 1TCO-A-B | 1THJ-B-C |
| 1TLF-A-B | 1TME-2-3 | 1TVX-B-D | 1UDI-E-I | 1VHI-A-B | 1VSC-A-B |
| 1WFB-A-B | 1XIK-A-B | 1YHA-A-B | 1YRN-A-B | 2ACH-A-B | 2BBV-B-C |
| 2CCY-A-B | 2DLD-A-B | 2KAU-A-C | 2LTN-A-B | 2MEV-2-3 | 2PKA-A-B |
| 3MDE-A-B | 3SIC-E-I | 4CHA-A-B | 4KBP-B-C | 6PFK-C-D | 9LDT-A-B |
| 1AHS-B-C | 1APY-A-B | 1BBH-A-B | 1BGL-A-D | 1BNC-A-B | 1CAX-C-F |
| 1CLX-A-B | 1DBQ-A-B | 1DPR-A-B | 1ECZ-A-B | 1EXT-A-B | 1FCD-B-D |
| 1FOD-1-3 | 1FUG-A-B | 1GES-A-B | 1GPM-B-D | 1HBH-C-D | 1HLE-A-B |
| 1HTR-B-P | 1HYL-A-B | 1KIF-B-F | 1LMK-E-G | 1LYL-A-C | 1MEE-A-I |
| 1MMO-C-H | 1MYK-A-B | 1NIP-A-B | 1OTF-B-E | 1PGE-A-B | 1POX-A-B |
| 1PRT-H-L | 1PVD-A-B | 1QOR-A-B | 1RHG-A-C | 1SCM-A-B | 1SLU-A-B |
| 1STM-B-C | 1TCR-A-B | 1TME-1-2 | 1TPH-1-2 | 1UBS-A-B | 1VOK-A-B |
| 1WHT-A-B | 1YPP-A-B | 2AFN-B-C | 2CHT-D-E | 2HNT-C-F | 2LTN-A-C |
| 2PEL-B-C | 2RSL-A-B | 2UTG-A-B | 3MON-C-D | 4CTS-A-B | 6FAB-H-L |

Supplementary material: Table 8. PDB identifiers and chain names for the test set of protein complexes.

| | | | | | |
|---|---|---|---|---|---|
| 1ACB-E-I | 1ATN-A-D | 1BBT-2-3 | 1BLB-A-B | 1BRS-C-F | 1CHM-A-B |
| 1CSM-A-B | 1DIR-A-B | 1ECF-A-B | 1EPT-A-B | 1FIN-A-B | 1FRT-A-C |
| 1GAD-O-P | 1GLQ-A-B | 1GTO-B-C | 1HGE-C-D | 1HRD-B-C | 1HUL-A-B |
| 1IES-B-E | 1KPT-A-B | 1LUC-A-B | 1MDA-H-L | 1MLD-A-B | 1MPM-B-C |
| 1NSC-A-B | 1ORO-A-B | 1OVA-C-D | 1PMA-C-D | 1PPF-E-I | 1PRE-A-B |
| 1PVC-1-2 | 1PYI-A-B | 1RBA-A-B | 1RVA-A-B | 1SET-A-B | 1SPB-P-S |
| 1TAF-A-B | 1TII-A-C | 1TMF-1-3 | 1TSR-A-B | 1UNA-A-B | 1VSG-A-B |
| 1XIM-A-C | 1YTF-B-D | 2BPA-1-3 | 2EIP-A-B | 2KAU-B-C | 2NAC-A-B |
| 2PLV-1-4 | 2SPC-A-B | 3HHR-A-B | 4AAH-A-C | 4SBV-A-B | 8ATC-A-B |