# Supplementary information 

Hai-Ping Sun, Yan Huang, Xiao-Fan Wang, Yang Zhang and Hong-Bin Shen, Improving accuracy of protein contact prediction using balanced network deconvolution

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Table S1. Edge weights in an 8 by 8 constructed symmetric matrix by ND and

## BND models (Fig.1c in the text).

| Node ID | Node ID | Original Edge weight | Edge weight rebuilt by ND noise model | Edge weight rebuilt by BND noise model |
| :---: | :---: | :---: | :---: | :---: |
| 1 | 2 | 0 | $2.95 \mathrm{E}+13$ | $3.69 \mathrm{E}+12$ |
| 1 | 3 | 0 | $2.23 \mathrm{E}+13$ | $1.95 \mathrm{E}+13$ |
| 1 | 4 | 0 | $1.67 \mathrm{E}+14$ | $2.08 \mathrm{E}+13$ |
| 1 | 5 | 0.369257 | 7.93E+14 | $6.94 \mathrm{E}+14$ |
| 1 | 6 | 0.597762 | $3.46 \mathrm{E}+14$ | $3.03 \mathrm{E}+14$ |
| 1 | 7 | 0 | $6.87 \mathrm{E}+14$ | $8.59 \mathrm{E}+13$ |
| 1 | 8 | 0 | $2.56 \mathrm{E}+13$ | $2.24 \mathrm{E}+13$ |
| 2 | 3 | 0.757482 | $1.32 \mathrm{E}+12$ | $1.15 \mathrm{E}+12$ |
| 2 | 4 | 0 | $9.83 \mathrm{E}+12$ | $1.23 \mathrm{E}+12$ |
| 2 | 5 | 0 | $4.68 \mathrm{E}+13$ | $4.09 \mathrm{E}+13$ |
| 2 | 6 | 0 | $2.04 \mathrm{E}+13$ | $1.79 \mathrm{E}+13$ |
| 2 | 7 | 0 | $4.05 \mathrm{E}+13$ | $5.06 \mathrm{E}+12$ |
| 2 | 8 | 0.490291 | $1.51 \mathrm{E}+12$ | $1.32 \mathrm{E}+12$ |
| 3 | 4 | 0 | $7.45 \mathrm{E}+12$ | $6.52 \mathrm{E}+12$ |
| 3 | 5 | 0 | $3.54 \mathrm{E}+13$ | $4.43 \mathrm{E}+12$ |
| 3 | 6 | 0 | $1.55 \mathrm{E}+13$ | $1.93 \mathrm{E}+12$ |
| 3 | 7 | 0 | $3.07 \mathrm{E}+13$ | $2.69 \mathrm{E}+13$ |
| 3 | 8 | 0 | $1.15 \mathrm{E}+12$ | $1.43 \mathrm{E}+11$ |
| 4 | 5 | 0.086159 | $2.65 \mathrm{E}+14$ | $2.31 \mathrm{E}+14$ |
| 4 | 6 | 0.284088 | $1.15 \mathrm{E}+14$ | $1.01 \mathrm{E}+14$ |
| 4 | 7 | 0 | $2.29 \mathrm{E}+14$ | $2.86 \mathrm{E}+13$ |
| 4 | 8 | 0 | $8.55 \mathrm{E}+12$ | $7.48 \mathrm{E}+12$ |
| 5 | 6 | 0 | $5.49 \mathrm{E}+14$ | $6.87 \mathrm{E}+13$ |
| 5 | 7 | 0.865322 | $1.09 \mathrm{E}+15$ | $9.54 \mathrm{E}+14$ |
| 5 | 8 | 0 | $4.07 \mathrm{E}+13$ | $5.08 \mathrm{E}+12$ |
| 6 | 7 | 0 | $4.76 \mathrm{E}+14$ | $4.16 \mathrm{E}+14$ |
| 6 | 8 | 0 | $1.77 \mathrm{E}+13$ | $2.22 \mathrm{E}+12$ |
| 7 | 8 | 0.016268 | $3.52 \mathrm{E}+13$ | $3.08 \mathrm{E}+13$ |

Table S2. Results for predicting protein residue contact maps on the CASP9
dataset.

Part 1 MI

| Evaluation methods | Predictors | \|i-j|>23 | 24>\|i-j|>11 | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 10.39\% | 8.88\% | 9.45\% | 11.93\% |
|  | MI+ND | 21.60\% | 18.24\% | 18.15\% | 25.50\% |
|  | MI + BND | 26.29\% | 22.49\% | 21.15\% | 31.23\% |
| Top L/5 | MI | 8.41\% | 7.48\% | 8.42\% | 10.32\% |
|  | MI + ND | 17.73\% | 14.44\% | 14.86\% | 21.95\% |
|  | MI+BND | 21.58\% | 17.53\% | 16.87\% | 26.99\% |
| Top L/2 | MI | 6.12\% | 6.37\% | 7.62\% | 8.28\% |
|  | MI+ND | 12.95\% | 10.47\% | 11.37\% | 16.76\% |
|  | MI + BND | 15.49\% | 12.21\% | 12.61\% | 20.08\% |
| Top $L$ | MI | 5.16\% | 5.41\% | 6.90\% | 6.96\% |
|  | MI+ND | 10.05\% | 8.18\% | 9.07\% | 13.18\% |
|  | MI + BND | 11.86\% | 9.32\% | 9.79\% | 15.66\% |

## Part 2 MIp

| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MIp | 10.39\% | 8.79\% | 9.57\% | 11.74\% |
|  | MIp+ND | 22.22\% | 17.73\% | 18.23\% | 25.30\% |
|  | MIp+BND | 26.49\% | 21.93\% | 21.11\% | 30.46\% |
| Top L/5 | MIp | 8.46\% | 7.37\% | 8.49\% | 10.26\% |
|  | MIp+ND | 18.13\% | 14.39\% | 15.32\% | 22.15\% |
|  | MIp+BND | 21.26\% | 17.43\% | 16.55\% | 26.57\% |
| Top $L / 2$ | MIp | 6.16\% | 6.41\% | 7.65\% | 8.31\% |
|  | MIp+ND | 13.19\% | 10.72\% | 11.60\% | 16.94\% |
|  | MIp+BND | 15.81\% | 12.52\% | 12.52\% | 19.86\% |
| Top L | MIp | 5.19\% | 5.38\% | 6.95\% | 7.01\% |
|  | MIp+ND | 10.25\% | 8.28\% | 9.21\% | 13.34\% |
|  | MIp+BND | 12.38\% | 9.71\% | 10.09\% | 15.72\% |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\|\mathbf{i}-\mathbf{j}\|>\mathbf{1 1}$ | $\mathbf{1 2}>\|\mathbf{i}-\mathbf{j}\|>\mathbf{5}$ | $\|\mathbf{i - j}\|>\mathbf{5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top $L / 10$ | DCA | $29.88 \%$ | $24.76 \%$ | $20.33 \%$ | $31.89 \%$ |
|  | DCA+ND | $29.86 \%$ | $24.51 \%$ | $22.72 \%$ | $32.81 \%$ |
|  | DCA+BND | $31.34 \%$ | $25.68 \%$ | $23.57 \%$ | $35.00 \%$ |


| Top $L / 5$ | DCA | $24.93 \%$ | $18.76 \%$ | $16.93 \%$ | $27.11 \%$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | DCA+ND | $25.59 \%$ | $19.52 \%$ | $18.29 \%$ | $28.82 \%$ |
|  | DCA+BND | $26.34 \%$ | $20.84 \%$ | $19.53 \%$ | $31.10 \%$ |
|  | DCA | $17.69 \%$ | $12.65 \%$ | $12.70 \%$ | $21.58 \%$ |
|  | DCA+ND | $17.82 \%$ | $13.07 \%$ | $13.33 \%$ | $22.76 \%$ |
| Top $L$ | DCA+BND | $18.87 \%$ | $14.05 \%$ | $14.28 \%$ | $23.96 \%$ |
|  | DCA | $12.71 \%$ | $9.19 \%$ | $9.97 \%$ | $16.88 \%$ |
|  | DCA+ND | $13.24 \%$ | $9.64 \%$ | $10.60 \%$ | $17.40 \%$ |
|  | DCA+BND | $14.00 \%$ | $10.34 \%$ | $11.02 \%$ | $18.72 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | $\|\mathrm{i}-\mathrm{j}\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 31.94\% | 23.33\% | 22.14\% | 36.18\% |
|  | PSICOV+ND | 31.57\% | 22.26\% | 22.39\% | 36.22\% |
|  | PSICOV+BND | 33.70\% | 24.70\% | 24.92\% | 40.07\% |
| Top L/5 | PSICOV | 25.02\% | 17.88\% | 17.70\% | 29.41\% |
|  | PSICOV+ND | 24.47\% | 17.16\% | 17.29\% | 30.46\% |
|  | PSICOV+BND | 26.21\% | 18.89\% | 18.97\% | 33.24\% |
| Top L/2 | PSICOV | 17.53\% | 12.64\% | 13.09\% | 21.80\% |
|  | PSICOV+ND | 16.35\% | 11.91\% | 12.69\% | 21.83\% |
|  | PSICOV+BND | 17.38\% | 12.74\% | 13.51\% | 23.52\% |
| Top $L$ | PSICOV | 13.18\% | 9.93\% | 10.60\% | 16.81\% |
|  | PSICOV+ND | 12.21\% | 9.13\% | 10.10\% | 16.34\% |
|  | PSICOV+BND | 12.94\% | 9.69\% | 10.51\% | 17.55\% |

## Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 34.29\% | 25.98\% | 21.50\% | 36.36\% |
|  | gDCA+ND | 35.32\% | 25.87\% | 20.89\% | 34.91\% |
|  | gDCA+BND | 35.87\% | 27.06\% | 22.27\% | 38.05\% |
| Top $L / 5$ | gDCA | 27.66\% | 20.75\% | 18.96\% | 31.18\% |
|  | gDCA+ND | 28.57\% | 20.39\% | 17.64\% | 30.30\% |
|  | gDCA+BND | 29.06\% | 20.87\% | 18.17\% | 32.56\% |
| Top L/2 | gDCA | 20.71\% | 14.55\% | 14.32\% | 23.59\% |
|  | gDCA+ND | 20.02\% | 14.25\% | 13.63\% | 23.41\% |
|  | gDCA+BND | 20.10\% | 13.88\% | 14.37\% | 24.36\% |
| Top $L$ | gDCA | 15.23\% | 10.98\% | 11.24\% | 18.83\% |
|  | gDCA+ND | 14.89\% | 10.49\% | 10.95\% | 18.53\% |
|  | gDCA+BND | 14.68\% | 10.35\% | 10.93\% | 18.75\% |

Table S3. Results for predicting protein residue contact maps on the CASP10
dataset.

Part 1 MI

| Evaluation methods | Predictors | $\|i-j\|>23$ | 24>\|i-j|>11 | 12>\|i-j|>5 | $\|\mathrm{i}-\mathrm{j}\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 15.82\% | 17.42\% | 13.97\% | 19.36\% |
|  | MI+ND | 30.63\% | 33.12\% | 25.12\% | 38.60\% |
|  | MI + BND | 36.78\% | 37.06\% | 28.60\% | 42.75\% |
| Top L/5 | MI | 13.82\% | 13.33\% | 11.85\% | 16.12\% |
|  | MI + ND | 25.45\% | 26.72\% | 19.68\% | 32.83\% |
|  | MI+BND | 30.77\% | 29.83\% | 22.05\% | 37.72\% |
| Top L/2 | MI | 9.97\% | 9.96\% | 9.97\% | 13.01\% |
|  | MI+ND | 18.89\% | 18.83\% | 14.55\% | 25.71\% |
|  | MI+BND | 22.63\% | 21.17\% | 16.14\% | 29.38\% |
| Top $L$ | MI | 7.71\% | 8.13\% | 8.20\% | 10.53\% |
|  | MI+ND | 14.15\% | 13.95\% | 11.14\% | 20.15\% |
|  | MI+BND | 16.69\% | 15.55\% | 12.07\% | 23.23\% |

Part 2 MIp

| Evaluation <br> methods | Predictors | $\|\mathbf{i} \mathbf{i} \mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\|\mathbf{i}-\mathbf{j}\| \mathbf{\mathbf { 1 1 }}$ | $\mathbf{1 2 >}>\mathbf{i} \mathbf{i} \mathbf{j} \mid>\mathbf{5}$ | $\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ |
| :---: | :--- | ---: | ---: | ---: | ---: |
| Top $L / 10$ | MIp | $15.82 \%$ | $17.42 \%$ | $14.06 \%$ | $19.36 \%$ |
|  | MIp+ND | $30.81 \%$ | $33.23 \%$ | $24.92 \%$ | $38.70 \%$ |
|  | MIp+BND | $36.53 \%$ | $36.69 \%$ | $28.29 \%$ | $42.83 \%$ |
| Top $L / 5$ | MIp | $13.82 \%$ | $13.40 \%$ | $11.90 \%$ | $16.31 \%$ |
|  | MIp+ND | $25.77 \%$ | $26.88 \%$ | $19.85 \%$ | $33.22 \%$ |
|  | MIp+BND | $30.99 \%$ | $29.72 \%$ | $22.11 \%$ | $37.05 \%$ |
|  | MIp | $10.02 \%$ | $9.97 \%$ | $10.27 \%$ | $13.03 \%$ |
|  | MIp+ND | $19.24 \%$ | $18.98 \%$ | $14.62 \%$ | $25.76 \%$ |
|  | MIp+BND | $22.88 \%$ | $21.31 \%$ | $16.17 \%$ | $29.38 \%$ |
|  | MIp | $7.69 \%$ | $8.05 \%$ | $8.36 \%$ | $10.56 \%$ |
| Top $L$ | MIp+ND | $14.32 \%$ | $14.14 \%$ | $11.27 \%$ | $20.33 \%$ |
|  | MIp+BND | $16.98 \%$ | $15.81 \%$ | $12.31 \%$ | $23.31 \%$ |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\mathbf{i} \mathbf{i} \mathbf{j} \mid>\mathbf{1 1}$ | $\mathbf{1 2}>\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ | $\|\mathbf{i} \mathbf{i} \mathbf{j}\|>\mathbf{5}$ |
| :---: | :--- | :---: | ---: | ---: | ---: |
| Top $L / 10$ | DCA | $40.74 \%$ | $39.56 \%$ | $29.50 \%$ | $44.06 \%$ |
|  | DCA+ND | $38.98 \%$ | $39.10 \%$ | $32.00 \%$ | $46.07 \%$ |
|  | DCA+BND | $41.42 \%$ | $40.04 \%$ | $33.80 \%$ | $48.94 \%$ |


| Top $L / 5$ | DCA | $34.48 \%$ | $32.30 \%$ | $23.88 \%$ | $39.66 \%$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | DCA+ND | $34.24 \%$ | $33.23 \%$ | $25.88 \%$ | $41.83 \%$ |
|  | DCA+BND | $35.62 \%$ | $33.83 \%$ | $27.17 \%$ | $43.78 \%$ |
|  | DCA | $25.94 \%$ | $22.81 \%$ | $16.73 \%$ | $33.00 \%$ |
| Top $L / 2$ | DCA+ND | $25.96 \%$ | $23.11 \%$ | $17.16 \%$ | $34.73 \%$ |
|  | DCA+BND | $26.80 \%$ | $24.02 \%$ | $17.74 \%$ | $36.14 \%$ |
|  | DCA | $19.13 \%$ | $16.55 \%$ | $12.38 \%$ | $26.71 \%$ |
|  | DCA+ND | $18.79 \%$ | $16.83 \%$ | $12.24 \%$ | $28.01 \%$ |
|  | DCA+BND | $19.51 \%$ | $17.39 \%$ | $12.62 \%$ | $29.11 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 41.45\% | 41.61\% | 31.57\% | 51.58\% |
|  | PSICOV+ND | 39.89\% | 40.73\% | 30.80\% | 50.56\% |
|  | PSICOV+BND | 41.55\% | 40.66\% | 33.48\% | 51.48\% |
| Top L/5 | PSICOV | 35.87\% | 32.63\% | 24.69\% | 44.82\% |
|  | PSICOV+ND | 34.75\% | 31.33\% | 23.84\% | 44.48\% |
|  | PSICOV+BND | 36.50\% | 32.28\% | 24.96\% | 46.47\% |
| Top $L / 2$ | PSICOV | 26.72\% | 22.55\% | 17.04\% | 35.57\% |
|  | PSICOV+ND | 24.81\% | 20.91\% | 16.10\% | 34.97\% |
|  | PSICOV+BND | 25.99\% | 21.87\% | 16.50\% | 36.18\% |
| Top L | PSICOV | 18.90\% | 16.63\% | 12.86\% | 27.67\% |
|  | PSICOV+ND | 17.14\% | 15.06\% | 11.75\% | 26.49\% |
|  | PSICOV+BND | 17.94\% | 15.99\% | 12.04\% | 27.47\% |

Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 45.22\% | 44.61\% | 34.05\% | 51.56\% |
|  | gDCA+ND | 42.78\% | 42.89\% | 33.51\% | 51.43\% |
|  | gDCA+BND | 45.13\% | 44.14\% | 35.42\% | 52.72\% |
| Top L/5 | gDCA | 40.11\% | 36.95\% | 27.29\% | 47.07\% |
|  | gDCA+ND | 38.26\% | 34.30\% | 27.00\% | 47.32\% |
|  | gDCA+BND | 39.67\% | 36.23\% | 27.70\% | 48.54\% |
| Top L/2 | gDCA | 30.36\% | 25.53\% | 18.60\% | 39.19\% |
|  | gDCA+ND | 27.57\% | 23.28\% | 17.22\% | 38.52\% |
|  | gDCA+BND | 29.35\% | 24.42\% | 18.20\% | 40.06\% |
| Top $L$ | gDCA | 22.25\% | 18.38\% | 13.53\% | 31.17\% |
|  | gDCA+ND | 19.16\% | 16.84\% | 12.51\% | 29.47\% |
|  | gDCA+BND | 20.65\% | 17.78\% | 12.99\% | 31.17\% |

Table S4. Results for predicting protein residue contact maps on the hard targets
in CASP9 dataset.

Part 1 MI

| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 7.62\% | 5.46\% | 7.32\% | 10.08\% |
|  | MI + ND | 14.47\% | 13.07\% | 13.99\% | 18.37\% |
|  | MI + BND | 20.53\% | 18.13\% | 19.20\% | 27.02\% |
| Top L/5 | MI | 6.59\% | 4.45\% | 6.62\% | 8.17\% |
|  | MI+ND | 13.04\% | 9.25\% | 12.37\% | 15.27\% |
|  | MI + BND | 16.41\% | 13.31\% | 14.54\% | 23.25\% |
| Top L/2 | MI | 4.81\% | 4.51\% | 6.14\% | 5.72\% |
|  | MI + ND | 9.68\% | 7.31\% | 9.68\% | 12.02\% |
|  | MI+BND | 12.10\% | 9.35\% | 10.80\% | 16.80\% |
| Top $L$ | MI | 4.04\% | 4.51\% | 6.05\% | 5.05\% |
|  | MI + ND | 7.45\% | 6.37\% | 7.84\% | 9.73\% |
|  | MI+BND | 9.01\% | 7.46\% | 8.48\% | 12.43\% |

Part 2 MIp

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i \mathbf{j}\|>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MIp | 7.62\% | 5.46\% | 7.32\% | 10.25\% |
|  | MIp+ND | 15.38\% | 12.26\% | 15.37\% | 18.63\% |
|  | MIp+BND | 20.88\% | 17.66\% | 20.01\% | 26.77\% |
| Top L/5 | MIp | 6.59\% | 4.45\% | 6.62\% | 8.17\% |
|  | MIp+ND | 13.33\% | 9.29\% | 13.16\% | 15.22\% |
|  | MIp+BND | 15.75\% | 13.67\% | 14.83\% | 22.76\% |
| Top $L / 2$ | MIp | 4.81\% | 4.56\% | 6.22\% | 5.72\% |
|  | MIp+ND | 9.93\% | 7.54\% | 10.22\% | 12.27\% |
|  | MIp+BND | 12.14\% | 9.65\% | 10.85\% | 16.49\% |
| Top $L$ | MIp | 4.04\% | 4.43\% | 6.15\% | 5.10\% |
|  | MIp+ND | 7.44\% | 6.39\% | 7.94\% | 10.00\% |
|  | MIp+BND | 9.23\% | 7.91\% | 8.74\% | 12.68\% |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\|\mathbf{i}-\mathbf{j}\|>\mathbf{1 1}$ | $\mathbf{1 2}>\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ | $\|\mathbf{i - j}\|>\mathbf{5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top $L / 10$ | DCA | $25.61 \%$ | $17.61 \%$ | $19.23 \%$ | $28.14 \%$ |
|  | DCA+ND | $26.04 \%$ | $16.79 \%$ | $21.49 \%$ | $27.49 \%$ |
|  | DCA+BND | $24.56 \%$ | $16.58 \%$ | $21.32 \%$ | $27.51 \%$ |


| Top $L / 5$ | DCA | $19.96 \%$ | $12.94 \%$ | $14.54 \%$ | $22.77 \%$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | DCA+ND | $19.75 \%$ | $13.12 \%$ | $15.92 \%$ | $23.50 \%$ |
|  | DCA+BND | $19.88 \%$ | $14.48 \%$ | $16.33 \%$ | $25.37 \%$ |
|  | DCA | $12.43 \%$ | $8.39 \%$ | $10.47 \%$ | $17.30 \%$ |
|  | DCA+ND | $12.60 \%$ | $9.16 \%$ | $10.55 \%$ | $17.49 \%$ |
| Top $L$ | DCA+BND | $13.26 \%$ | $10.24 \%$ | $11.91 \%$ | $18.60 \%$ |
|  | DCA | $8.62 \%$ | $6.64 \%$ | $8.22 \%$ | $12.51 \%$ |
|  | DCA+ND | $9.37 \%$ | $7.25 \%$ | $8.78 \%$ | $12.75 \%$ |
|  | DCA+BND | $10.09 \%$ | $8.02 \%$ | $9.24 \%$ | $13.88 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | $\|\mathrm{i}-\mathrm{j}\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 23.43\% | 17.73\% | 18.14\% | 29.78\% |
|  | PSICOV+ND | 22.63\% | 16.54\% | 17.68\% | 29.00\% |
|  | PSICOV+BND | 24.44\% | 17.33\% | 18.14\% | 30.63\% |
| Top L/5 | PSICOV | 17.35\% | 13.86\% | 14.14\% | 22.95\% |
|  | PSICOV+ND | 16.61\% | 12.53\% | 13.15\% | 22.44\% |
|  | PSICOV+BND | 17.19\% | 12.85\% | 13.79\% | 24.25\% |
| Top $L / 2$ | PSICOV | 12.72\% | 9.47\% | 10.95\% | 15.79\% |
|  | PSICOV+ND | 11.74\% | 9.19\% | 9.92\% | 15.60\% |
|  | PSICOV+BND | 12.91\% | 10.13\% | 11.30\% | 16.18\% |
| Top $L$ | PSICOV | 9.59\% | 8.21\% | 8.81\% | 12.99\% |
|  | PSICOV+ND | 9.20\% | 7.59\% | 8.45\% | 12.13\% |
|  | PSICOV+BND | 9.32\% | 8.06\% | 9.08\% | 13.20\% |

Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i \mathbf{i}\|>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 29.30\% | 20.52\% | 18.57\% | 31.13\% |
|  | gDCA+ND | 29.55\% | 16.61\% | 17.68\% | 29.02\% |
|  | gDCA+BND | 29.53\% | 18.99\% | 18.91\% | 32.01\% |
| Top L/5 | gDCA | 21.75\% | 15.75\% | 16.54\% | 26.98\% |
|  | gDCA+ND | 22.11\% | 13.74\% | 15.72\% | 24.63\% |
|  | gDCA+BND | 21.84\% | 14.79\% | 15.33\% | 25.81\% |
| Top L/2 | gDCA | 15.16\% | 11.10\% | 11.68\% | 19.22\% |
|  | gDCA+ND | 13.97\% | 10.83\% | 11.41\% | 19.01\% |
|  | gDCA+BND | 13.57\% | 10.23\% | 12.09\% | 18.65\% |
| Top $L$ | gDCA | 11.32\% | 8.14\% | 9.76\% | 15.24\% |
|  | gDCA+ND | 10.78\% | 7.64\% | 9.49\% | 14.56\% |
|  | gDCA+BND | 10.58\% | 7.82\% | 9.71\% | 14.11\% |

Table S5. Results for predicting protein residue contact maps on the hard targets
in CASP10 dataset.

Part 1 MI

| Evaluation methods | Predictors | $\|i-j\|>23$ | 24>\|i-j|>11 | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 9.48\% | 12.60\% | 7.71\% | 10.88\% |
|  | MI+ND | 13.89\% | 21.72\% | 13.35\% | 19.99\% |
|  | MI + BND | 18.61\% | 23.47\% | 17.55\% | 24.09\% |
| Top L/5 | MI | 8.27\% | 9.78\% | 7.05\% | 8.83\% |
|  | MI + ND | 12.04\% | 17.81\% | 10.48\% | 16.84\% |
|  | MI+BND | 15.72\% | 19.66\% | 13.21\% | 20.91\% |
| Top L/2 | MI | 6.54\% | 6.98\% | 6.34\% | 7.33\% |
|  | MI+ND | 9.09\% | 12.63\% | 8.87\% | 13.12\% |
|  | MI+BND | 11.28\% | 14.61\% | 10.31\% | 15.25\% |
| Top $L$ | MI | 5.35\% | 5.81\% | 5.69\% | 6.29\% |
|  | MI+ND | 7.07\% | 10.47\% | 7.84\% | 10.35\% |
|  | MI+BND | 8.82\% | 11.79\% | 8.74\% | 12.04\% |

## Part 2 MIp

| Part 2 MIp |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| Top L/10 | MIp | 9.48\% | 12.60\% | 7.71\% | 10.88\% |
|  | MIp+ND | 13.99\% | 21.26\% | 13.66\% | 20.70\% |
|  | MIp+BND | 17.83\% | 22.62\% | 17.16\% | 24.09\% |
| Top L/5 | MIp | 8.27\% | 10.18\% | 7.05\% | 9.33\% |
|  | MIp+ND | 12.04\% | 18.10\% | 11.08\% | 17.08\% |
|  | MIp+BND | 16.59\% | 19.89\% | 13.47\% | 20.51\% |
| Top $L / 2$ | MIp | 6.70\% | 6.93\% | 7.28\% | 7.36\% |
|  | MIp+ND | 9.61\% | 12.79\% | 9.03\% | 13.20\% |
|  | MIp+BND | 11.76\% | 14.87\% | 10.71\% | 15.41\% |
| Top $L$ | MIp | 5.30\% | 5.70\% | 6.22\% | 6.40\% |
|  | MIp+ND | 7.32\% | 10.57\% | 7.71\% | 10.55\% |
|  | MIp+BND | 9.22\% | 12.00\% | 8.56\% | 12.44\% |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\mathbf{i} \mathbf{i} \mathbf{j} \mid>\mathbf{1 1}$ | $\mathbf{1 2}>\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ | $\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ |
| :---: | :--- | :---: | ---: | ---: | ---: |
| Top $L / 10$ | DCA | $19.08 \%$ | $22.89 \%$ | $17.09 \%$ | $22.94 \%$ |
|  | DCA+ND | $16.61 \%$ | $21.07 \%$ | $17.25 \%$ | $24.28 \%$ |
|  | DCA+BND | $20.30 \%$ | $23.74 \%$ | $18.71 \%$ | $28.53 \%$ |


| Top $L / 5$ | DCA | $14.34 \%$ | $18.87 \%$ | $12.93 \%$ | $20.77 \%$ |
| :--- | :--- | ---: | ---: | ---: | ---: |
|  | DCA+ND | $14.61 \%$ | $19.12 \%$ | $13.96 \%$ | $21.51 \%$ |
|  | DCA+BND | $15.67 \%$ | $19.61 \%$ | $15.45 \%$ | $23.85 \%$ |
|  | DCA | $11.44 \%$ | $14.74 \%$ | $9.51 \%$ | $16.57 \%$ |
| Top $L / 2$ | DCA+ND | $11.13 \%$ | $15.58 \%$ | $10.45 \%$ | $17.51 \%$ |
|  | DCA+BND | $11.74 \%$ | $16.19 \%$ | $10.87 \%$ | $18.72 \%$ |
|  | DCA | $9.16 \%$ | $11.88 \%$ | $7.94 \%$ | $13.06 \%$ |
|  | DCA+ND | $8.46 \%$ | $12.58 \%$ | $8.43 \%$ | $14.03 \%$ |
|  | DCA+BND | $8.75 \%$ | $13.28 \%$ | $8.97 \%$ | $14.78 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 17.58\% | 24.89\% | 15.62\% | 27.20\% |
|  | PSICOV+ND | 16.10\% | 24.12\% | 13.96\% | 27.49\% |
|  | PSICOV+BND | 19.09\% | 23.33\% | 15.82\% | 29.83\% |
| Top L/5 | PSICOV | 15.39\% | 18.77\% | 11.14\% | 21.90\% |
|  | PSICOV+ND | 14.11\% | 18.68\% | 11.45\% | 22.24\% |
|  | PSICOV+BND | 16.10\% | 18.81\% | 11.60\% | 24.37\% |
| Top $L / 2$ | PSICOV | 11.34\% | 14.65\% | 9.74\% | 16.89\% |
|  | PSICOV+ND | 10.66\% | 14.28\% | 9.49\% | 16.95\% |
|  | PSICOV+BND | 11.11\% | 15.38\% | 9.54\% | 17.38\% |
| Top L | PSICOV | 8.62\% | 12.01\% | 9.66\% | 13.13\% |
|  | PSICOV+ND | 7.93\% | 11.67\% | 9.10\% | 13.05\% |
|  | PSICOV+BND | 8.15\% | 11.94\% | 9.27\% | 13.94\% |

## Part 5 gDCA

| Evaluation methods | Predictors | $\|\mathrm{i}-\mathrm{j}\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 20.86\% | 27.05\% | 17.10\% | 27.90\% |
|  | gDCA+ND | 19.28\% | 22.49\% | 16.23\% | 27.39\% |
|  | gDCA+BND | 21.82\% | 25.23\% | 16.80\% | 28.65\% |
| Top L/5 | gDCA | 18.04\% | 21.73\% | 14.69\% | 23.79\% |
|  | gDCA+ND | 16.56\% | 19.99\% | 14.00\% | 24.35\% |
|  | gDCA+BND | 17.66\% | 21.35\% | 12.98\% | 25.67\% |
| Top $L / 2$ | gDCA | 13.31\% | 16.74\% | 10.73\% | 19.11\% |
|  | gDCA+ND | 11.42\% | 15.62\% | 10.69\% | 19.24\% |
|  | gDCA+BND | 12.48\% | 16.42\% | 10.73\% | 20.22\% |
| Top $L$ | gDCA | 10.24\% | 13.22\% | 9.46\% | 15.10\% |
|  | gDCA+ND | 8.68\% | 12.96\% | 9.03\% | 15.38\% |
|  | gDCA+BND | 9.36\% | 13.70\% | 9.02\% | 15.95\% |

Table S6. Results for predicting protein residue contact maps on the PSICOV
dataset.

Part 1 MI

| Evaluation methods | Predictors | $\|i-j\|>23$ | 24>\|i-j|>11 | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 29.12\% | 22.26\% | 19.83\% | 30.28\% |
|  | MI+ND | 55.04\% | 45.59\% | 39.74\% | 61.93\% |
|  | MI +BND | 60.76\% | 50.03\% | 43.11\% | 66.36\% |
| Top L/5 | MI | 23.15\% | 16.95\% | 16.17\% | 25.08\% |
|  | MI+ND | 46.89\% | 35.47\% | 30.37\% | 53.90\% |
|  | MI+BND | 52.23\% | 39.96\% | 33.28\% | 58.84\% |
| Top $L / 2$ | MI | 16.33\% | 12.39\% | 11.94\% | 18.71\% |
|  | MI+ND | 33.58\% | 22.41\% | 19.70\% | 42.11\% |
|  | MI +BND | 38.61\% | 25.77\% | 21.34\% | 46.19\% |
| Top $L$ | MI | 12.42\% | 9.32\% | 9.84\% | 15.50\% |
|  | MI+ND | 24.18\% | 15.15\% | 13.81\% | 31.83\% |
|  | MI + BND | 27.99\% | 17.19\% | 14.81\% | 35.57\% |

## Part 2 MIp

| Evaluation methods | Predictors | \|i-j|>23 | 24> $>$ i-j ${ }^{\text {l }}>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MIp | 29.12\% | 22.26\% | 19.83\% | 30.28\% |
|  | MIp+ND | 55.15\% | 45.68\% | 39.66\% | 62.07\% |
|  | MIp+BND | 60.20\% | 50.12\% | 43.29\% | 65.83\% |
| Top L/5 | MIp | 23.15\% | 16.95\% | 16.17\% | 25.08\% |
|  | MIp+ND | 46.96\% | 35.53\% | 30.60\% | 53.96\% |
|  | MIp+BND | 52.29\% | 40.03\% | 33.26\% | 58.87\% |
| Top L/2 | MIp | 16.33\% | 12.39\% | 11.94\% | 18.71\% |
|  | MIp+ND | 33.86\% | 22.60\% | 19.94\% | 42.21\% |
|  | MIp+BND | 38.73\% | 25.96\% | 21.57\% | 46.11\% |
| Top $L$ | MIp | 12.42\% | 9.32\% | 9.84\% | 15.50\% |
|  | MIp+ND | 24.35\% | 15.36\% | 13.88\% | 31.90\% |
|  | MIp+BND | 28.11\% | 17.25\% | 14.92\% | 35.59\% |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i - j} \mathbf{j}\|>\mathbf{2 3}$ | $\mathbf{2 4}>\|\mathbf{i} \mathbf{- j}\|>\mathbf{1 1}$ | $\mathbf{1 2}>\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ | $\|\mathbf{i} \mathbf{- j}\|>\mathbf{5}$ |
| :--- | :--- | :--- | ---: | ---: | ---: |
| Top $L / 10$ | DCA | $54.92 \%$ | $53.45 \%$ | $43.33 \%$ | $60.14 \%$ |
|  | DCA+ND | $56.06 \%$ | $54.89 \%$ | $46.37 \%$ | $63.57 \%$ |
|  | DCA+BND | $58.03 \%$ | $56.86 \%$ | $48.73 \%$ | $65.96 \%$ |


| Top $L / 5$ | DCA | $50.55 \%$ | $42.81 \%$ | $35.22 \%$ | $56.45 \%$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | DCA+ND | $51.42 \%$ | $44.30 \%$ | $36.86 \%$ | $58.66 \%$ |
|  | DCA+BND | $53.44 \%$ | $45.49 \%$ | $37.61 \%$ | $60.92 \%$ |
|  | DCA | $40.00 \%$ | $26.58 \%$ | $22.51 \%$ | $47.98 \%$ |
| Top $L / 2$ | DCA+ND | $40.81 \%$ | $27.04 \%$ | $22.61 \%$ | $49.92 \%$ |
|  | DCA+BND | $42.39 \%$ | $28.24 \%$ | $23.34 \%$ | $51.66 \%$ |
|  | DCA | $29.18 \%$ | $17.02 \%$ | $15.18 \%$ | $38.35 \%$ |
|  | DCA+ND | $29.58 \%$ | $17.00 \%$ | $14.60 \%$ | $39.81 \%$ |
|  | DCA+BND | $30.72 \%$ | $17.69 \%$ | $15.14 \%$ | $41.11 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | \|i-j|>23 | $24>\|i-j\|>11$ | 12> ${ }^{\text {i-j}} \mathbf{j} \mid>5$ | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 71.77\% | 58.11\% | 50.95\% | 77.11\% |
|  | PSICOV+ND | 70.53\% | 56.97\% | 49.72\% | 76.66\% |
|  | PSICOV+BND | 71.22\% | 57.60\% | 51.25\% | 77.03\% |
| Top L/5 | PSICOV | 62.56\% | 45.87\% | 38.62\% | 71.19\% |
|  | PSICOV+ND | 60.69\% | 43.27\% | 36.77\% | 70.28\% |
|  | PSICOV+BND | 62.42\% | 44.82\% | 38.06\% | 70.65\% |
| Top L/2 | PSICOV | 44.74\% | 27.81\% | 23.94\% | 56.22\% |
|  | PSICOV+ND | 42.10\% | 25.09\% | 21.68\% | 54.63\% |
|  | PSICOV+BND | 44.05\% | 26.29\% | 22.71\% | 56.39\% |
| Top $L$ | PSICOV | 31.48\% | 17.96\% | 16.12\% | 42.55\% |
|  | PSICOV+ND | 28.60\% | 15.87\% | 14.16\% | 39.87\% |
|  | PSICOV+BND | 29.91\% | 16.35\% | 14.82\% | 41.42\% |

Part 5 gDCA

| Evaluation methods | Predictors | \|i-j|>23 | 24>\|i-j|>11 | 12>\|i-j|>5 | $\|\mathrm{i}-\mathrm{j}\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 72.86\% | 60.79\% | 54.59\% | 76.56\% |
|  | gDCA+ND | 72.86\% | 61.51\% | 54.04\% | 78.73\% |
|  | gDCA+BND | 73.62\% | 62.96\% | 56.63\% | 78.52\% |
| Top L/5 | gDCA | 64.70\% | 50.28\% | 42.15\% | 71.81\% |
|  | gDCA+ND | 64.31\% | 47.48\% | 40.33\% | 72.11\% |
|  | gDCA+BND | 66.38\% | 50.16\% | 42.44\% | 73.86\% |
| Top L/2 | gDCA | 50.61\% | 31.81\% | 26.32\% | 59.94\% |
|  | gDCA+ND | 47.27\% | 28.24\% | 23.85\% | 59.04\% |
|  | gDCA+BND | 50.39\% | 30.19\% | 25.41\% | 61.59\% |
| Top $L$ | gDCA | 36.90\% | 20.51\% | 17.37\% | 47.72\% |
|  | gDCA+ND | 32.24\% | 17.71\% | 15.56\% | 44.25\% |
|  | gDCA+BND | 35.19\% | 19.02\% | 16.55\% | 47.42\% |

Table S7. Results for predicting protein residue contact maps on the CASP9
dataset at different cutoff values of long-range contacts.

Part 1 MI

| Evaluation methods | Predictors | \|i-j|>23 | \|i-j|>20 | $\|\mathrm{i}-\mathrm{j}\|>15$ | \|i-j|>8 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 10.39\% | 10.68\% | 10.68\% | 11.59\% |
|  | MI+ND | 21.60\% | 22.26\% | 23.28\% | 25.19\% |
|  | MI + BND | 26.29\% | 27.66\% | 28.81\% | 31.44\% |
| Top $L / 5$ | MI | 8.41\% | 8.58\% | 9.09\% | 10.03\% |
|  | MI+ND | 17.73\% | 18.68\% | 19.65\% | 21.50\% |
|  | MI + BND | 21.58\% | 22.40\% | 23.49\% | 26.34\% |
| Top $L / 2$ | MI | 6.12\% | 6.51\% | 6.98\% | 7.58\% |
|  | MI+ND | 12.95\% | 13.43\% | 14.22\% | 16.16\% |
|  | MI+BND | 15.49\% | 16.38\% | 17.36\% | 19.37\% |
| Top L | MI | 5.16\% | 5.43\% | 5.82\% | 6.47\% |
|  | MI + ND | 10.05\% | 10.52\% | 11.31\% | 12.47\% |
|  | MI +BND | 11.86\% | 12.55\% | 13.39\% | 14.90\% |

## Part 2 MIp

| Evaluation methods | Predictors | $\|i-j\|>23$ | \|i-j|>20 | \|i-j|>15 | $\|\mathrm{i}-\mathrm{j}\|>8$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MIp | 10.39\% | 10.68\% | 10.68\% | 11.37\% |
|  | MIp+ND | 22.22\% | 22.64\% | 23.56\% | 25.28\% |
|  | MIp+BND | 26.49\% | 27.24\% | 28.80\% | 30.40\% |
| Top L/5 | MIp | 8.46\% | 8.66\% | 9.06\% | 9.94\% |
|  | MIp+ND | 18.13\% | 18.79\% | 19.82\% | 21.64\% |
|  | MIp+BND | 21.26\% | 22.74\% | 23.36\% | 25.75\% |
| Top $L / 2$ | MIp | 6.16\% | 6.54\% | 6.95\% | 7.60\% |
|  | MIp+ND | 13.19\% | 13.80\% | 14.59\% | 16.23\% |
|  | MIp+BND | 15.81\% | 16.50\% | 17.50\% | 19.45\% |
| Top L | MIp | 5.19\% | 5.44\% | 5.82\% | 6.44\% |
|  | MIp+ND | 10.25\% | 10.76\% | 11.43\% | 12.58\% |
|  | MIp+BND | 12.38\% | 12.96\% | 13.79\% | 14.99\% |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 0}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{1 5}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{8}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top $L / 10$ | DCA | $29.88 \%$ | $30.49 \%$ | $31.21 \%$ | $33.19 \%$ |
|  | DCA+ND | $29.86 \%$ | $30.51 \%$ | $31.80 \%$ | $33.90 \%$ |
|  | DCA+BND | $31.34 \%$ | $31.42 \%$ | $32.89 \%$ | $35.67 \%$ |


| Top $L / 5$ | DCA | $24.93 \%$ | $25.81 \%$ | $26.75 \%$ | $27.82 \%$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | DCA+ND | $25.59 \%$ | $26.46 \%$ | $27.56 \%$ | $28.58 \%$ |
|  | DCA+BND | $26.34 \%$ | $27.32 \%$ | $28.64 \%$ | $30.86 \%$ |
|  | DCA | $17.69 \%$ | $18.61 \%$ | $19.73 \%$ | $21.63 \%$ |
|  | DCA+ND | $17.82 \%$ | $18.78 \%$ | $20.13 \%$ | $22.14 \%$ |
| Top $L$ | DCA+BND | $18.87 \%$ | $19.75 \%$ | $21.30 \%$ | $23.24 \%$ |
|  | DCA | $12.71 \%$ | $13.50 \%$ | $14.59 \%$ | $16.25 \%$ |
|  | DCA+ND | $13.24 \%$ | $13.87 \%$ | $14.93 \%$ | $16.64 \%$ |
|  | DCA+BND | $14.00 \%$ | $14.83 \%$ | $15.94 \%$ | $17.61 \%$ |

Part 4 PSICOV

| Evaluation methods | Predictors | \|i-j|>23 | $\|i-j\|>20$ | \|i-j|>15 | $\|\mathrm{i}-\mathrm{j}\|>8$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 31.94\% | 32.21\% | 33.90\% | 36.73\% |
|  | PSICOV+ND | 31.57\% | 31.99\% | 33.32\% | 36.70\% |
|  | PSICOV+BND | 33.70\% | 34.23\% | 35.89\% | 39.54\% |
| Top L/5 | PSICOV | 25.02\% | 26.28\% | 27.16\% | 29.76\% |
|  | PSICOV+ND | 24.47\% | 25.52\% | 26.88\% | 29.93\% |
|  | PSICOV+BND | 26.21\% | 27.58\% | 28.94\% | 32.62\% |
| Top $L / 2$ | PSICOV | 17.53\% | 18.56\% | 19.27\% | 20.97\% |
|  | PSICOV+ND | 16.35\% | 17.39\% | 18.50\% | 20.55\% |
|  | PSICOV+BND | 17.38\% | 18.19\% | 19.47\% | 22.22\% |
| Top $L$ | PSICOV | 13.18\% | 13.83\% | 14.70\% | 16.16\% |
|  | PSICOV+ND | 12.21\% | 12.62\% | 13.55\% | 15.27\% |
|  | PSICOV+BND | 12.94\% | 13.50\% | 14.38\% | 16.39\% |

## Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i \mathbf{j}\|>11$ | 12>\|i-j|>5 | $\|\mathrm{i}-\mathrm{j}\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 34.29\% | 35.67\% | 36.55\% | 38.02\% |
|  | gDCA+ND | 35.32\% | 35.67\% | 36.32\% | 37.44\% |
|  | gDCA+BND | 35.87\% | 36.57\% | 37.37\% | 39.63\% |
| Top L/5 | gDCA | 27.66\% | 28.95\% | 29.73\% | 32.23\% |
|  | gDCA+ND | 28.57\% | 29.68\% | 30.84\% | 32.18\% |
|  | gDCA+BND | 29.06\% | 30.17\% | 31.25\% | 33.90\% |
| Top L/2 | gDCA | 20.71\% | 21.43\% | 21.99\% | 23.65\% |
|  | gDCA+ND | 20.02\% | 21.15\% | 22.44\% | 23.99\% |
|  | gDCA+BND | 20.10\% | 20.99\% | 22.36\% | 24.39\% |
| Top $L$ | gDCA | 15.23\% | 16.09\% | 17.09\% | 18.36\% |
|  | gDCA+ND | 14.89\% | 15.64\% | 16.66\% | 18.13\% |
|  | gDCA+BND | 14.68\% | 15.56\% | 16.66\% | 18.22\% |

Table S8. Results for predicting protein residue contact maps on the CASP10
dataset at different cutoff values of long-range contacts.

Part 1 MI

| Evaluation methods | Predictors | $\|i-j\|>23$ | $\|i-j\|>20$ | $\|i-j\|>15$ | $\|\mathbf{i - j}\|>8$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 15.82\% | 18.81\% | 17.77\% | 19.77\% |
|  | MI+ND | 30.63\% | 35.39\% | 36.62\% | 40.60\% |
|  | MI +BND | 36.78\% | 39.65\% | 40.66\% | 44.97\% |
| Top L/5 | MI | 13.82\% | 16.30\% | 14.70\% | 16.78\% |
|  | MI+ND | 25.45\% | 29.22\% | 30.98\% | 33.80\% |
|  | MI + BND | 30.77\% | 34.33\% | 36.02\% | 39.24\% |
| Top $L / 2$ | MI | 9.97\% | 11.97\% | 11.68\% | 12.69\% |
|  | MI+ND | 18.89\% | 21.93\% | 23.71\% | 26.14\% |
|  | MI +BND | 22.63\% | 26.04\% | 27.79\% | 30.48\% |
| Top L | MI | 7.71\% | 9.67\% | 9.47\% | 9.84\% |
|  | MI+ND | 14.15\% | 17.05\% | 18.31\% | 20.03\% |
|  | MI+BND | 16.69\% | 19.61\% | 21.25\% | 23.36\% |

Part 2 MIp

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 0}$ | $\|\mathbf{i - j}\|>\mathbf{1 5}$ | $\|\mathbf{i - j} \mathbf{j}\|>\mathbf{8}$ |
| :---: | :--- | :--- | :---: | ---: | ---: |
| Top $L / 10$ | MIp | $15.82 \%$ | $18.81 \%$ | $17.77 \%$ | $19.86 \%$ |
|  | MIp+ND | $30.81 \%$ | $35.52 \%$ | $37.01 \%$ | $40.45 \%$ |
|  | MIp+BND | $36.53 \%$ | $39.63 \%$ | $40.81 \%$ | $45.05 \%$ |
| Top $L / 5$ | MIp | $13.82 \%$ | $16.30 \%$ | $14.82 \%$ | $16.99 \%$ |
|  | MIp+ND | $25.77 \%$ | $29.73 \%$ | $31.32 \%$ | $34.45 \%$ |
|  | MIp+BND | $30.99 \%$ | $34.81 \%$ | $36.00 \%$ | $39.16 \%$ |
|  | MIp | $10.02 \%$ | $11.97 \%$ | $11.68 \%$ | $12.69 \%$ |
|  | MIp+ND | $19.24 \%$ | $22.44 \%$ | $23.88 \%$ | $26.26 \%$ |
|  | MIp+BND | $22.88 \%$ | $26.49 \%$ | $28.44 \%$ | $30.67 \%$ |
|  | MIp | $7.69 \%$ | $9.66 \%$ | $9.43 \%$ | $9.99 \%$ |
| Top $L$ | MIp+ND | $14.32 \%$ | $17.26 \%$ | $18.68 \%$ | $20.33 \%$ |
|  | MIp+BND | $16.98 \%$ | $19.84 \%$ | $21.43 \%$ | $23.72 \%$ |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 0}$ | $\|\mathbf{i - j}\|>\mathbf{1 5}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{8}$ |
| :---: | :--- | :--- | :--- | :--- | :--- |
| Top $L / 10$ | DCA | $40.74 \%$ | $44.21 \%$ | $44.66 \%$ | $46.96 \%$ |
|  | DCA+ND | $38.98 \%$ | $42.98 \%$ | $44.49 \%$ | $47.13 \%$ |
|  | DCA+BND | $41.42 \%$ | $45.41 \%$ | $46.73 \%$ | $49.49 \%$ |


| Top $L / 5$ | DCA | $34.48 \%$ | $38.47 \%$ | $39.87 \%$ | $41.94 \%$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | DCA+ND | $34.24 \%$ | $38.98 \%$ | $39.92 \%$ | $42.08 \%$ |
|  | DCA+BND | $35.62 \%$ | $40.18 \%$ | $41.51 \%$ | $44.11 \%$ |
|  | DCA | $25.94 \%$ | $29.80 \%$ | $31.88 \%$ | $33.78 \%$ |
| Top $L / 2$ | DCA+ND | $25.96 \%$ | $30.04 \%$ | $31.81 \%$ | $34.36 \%$ |
|  | DCA+BND | $26.80 \%$ | $31.17 \%$ | $33.19 \%$ | $35.52 \%$ |
|  | DCA | $19.13 \%$ | $22.87 \%$ | $24.84 \%$ | $26.69 \%$ |
|  | DCA+ND | $18.79 \%$ | $22.55 \%$ | $24.59 \%$ | $27.27 \%$ |
|  | DCA+BND | $19.51 \%$ | $23.30 \%$ | $25.55 \%$ | $28.24 \%$ |

## Part 4 PSICOV

| Evaluation methods | Predictors | \|i-j|>23 | $\|i-j\|>20$ | \|i-j|>15 | $\|\mathrm{i}-\mathrm{j}\|>8$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 41.45\% | 45.29\% | 47.93\% | 52.01\% |
|  | PSICOV+ND | 39.89\% | 44.20\% | 46.70\% | 50.13\% |
|  | PSICOV+BND | 41.55\% | 45.46\% | 47.19\% | 50.99\% |
| Top L/5 | PSICOV | 35.87\% | 40.31\% | 41.40\% | 45.37\% |
|  | PSICOV+ND | 34.75\% | 39.23\% | 40.52\% | 44.21\% |
|  | PSICOV+BND | 36.50\% | 40.68\% | 42.74\% | 45.89\% |
| Top $L / 2$ | PSICOV | 26.72\% | 30.69\% | 33.03\% | 35.09\% |
|  | PSICOV+ND | 24.81\% | 29.12\% | 31.58\% | 34.08\% |
|  | PSICOV+BND | 25.99\% | 30.52\% | 32.59\% | 35.27\% |
| Top $L$ | PSICOV | 18.90\% | 22.26\% | 24.33\% | 26.72\% |
|  | PSICOV+ND | 17.14\% | 20.62\% | 22.58\% | 25.25\% |
|  | PSICOV+BND | 17.94\% | 15.99\% | 12.04\% | 27.47\% |

## Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | 24>\|i-j|>11 | 12>\|i-j|>5 | \|i-j|>5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 45.22\% | 47.87\% | 49.55\% | 51.77\% |
|  | gDCA+ND | 42.78\% | 46.16\% | 47.82\% | 50.89\% |
|  | gDCA+BND | 45.13\% | 47.99\% | 48.89\% | 51.87\% |
| Top L/5 | gDCA | 40.11\% | 44.07\% | 45.97\% | 47.68\% |
|  | gDCA+ND | 38.26\% | 42.79\% | 44.02\% | 46.96\% |
|  | gDCA+BND | 39.67\% | 44.08\% | 46.07\% | 48.32\% |
| Top L/2 | gDCA | 30.36\% | 34.74\% | 37.07\% | 39.32\% |
|  | gDCA+ND | 27.57\% | 32.17\% | 34.35\% | 37.38\% |
|  | gDCA+BND | 29.35\% | 33.74\% | 36.44\% | 39.22\% |
| Top $L$ | gDCA | 22.25\% | 26.33\% | 28.43\% | 30.74\% |
|  | gDCA+ND | 19.16\% | 23.26\% | 25.37\% | 28.21\% |
|  | gDCA+BND | 20.65\% | 24.67\% | 27.02\% | 30.15\% |

Table S9. Results for predicting protein residue contact maps on the PSICOV
dataset at different cutoff values of long-range contacts.

Part 1 MI

| Evaluation methods | Predictors | $\|i-j\|>23$ | \|i-j|>20 | $\|i-j\|>15$ | \|i-j|>8 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | MI | 29.12\% | 29.91\% | 32.40\% | 31.83\% |
|  | MI+ND | 55.04\% | 55.65\% | 58.04\% | 61.57\% |
|  | MI +BND | 60.76\% | 61.32\% | 64.08\% | 67.30\% |
| Top L/5 | MI | 23.15\% | 23.54\% | 24.73\% | 25.79\% |
|  | MI+ND | 46.89\% | 47.76\% | 50.19\% | 53.64\% |
|  | MI + BND | 52.23\% | 53.87\% | 56.63\% | 59.45\% |
| Top L/2 | MI | 16.33\% | 17.25\% | 18.40\% | 18.91\% |
|  | MI+ND | 33.58\% | 35.30\% | 37.59\% | 41.55\% |
|  | MI + BND | 38.61\% | 40.46\% | 43.21\% | 46.32\% |
| Top $L$ | MI | 12.42\% | 13.10\% | 14.03\% | 15.14\% |
|  | MI+ND | 24.18\% | 25.73\% | 27.72\% | 30.57\% |
|  | MI+BND | 27.99\% | 29.72\% | 31.95\% | 35.09\% |

Part 2 MIp

| Evaluation <br> methods | Predictors | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | $\|\mathbf{i} \mathbf{- j \|}\|>\mathbf{2 0}$ | $\|\mathbf{i - j}\|>\mathbf{1 5}$ | $\|\mathbf{i - j}\|>\mathbf{8}$ |
| :---: | :--- | :--- | :--- | :--- | :--- |
| Top $L / 10$ | MIp | MIp+ND | $29.12 \%$ | $29.91 \%$ | $32.40 \%$ |
|  | MIp+BND | $60.15 \%$ | $55.89 \%$ | $58.28 \%$ | $61.83 \%$ |
|  | MIp | $23.15 \%$ | $61.02 \%$ | $63.79 \%$ | $66.99 \%$ |
| Top $L / 5$ | MIp+ND | $46.96 \%$ | $47.96 \%$ | $24.73 \%$ | $25.79 \%$ |
|  | MIp+BND | $52.29 \%$ | $53.94 \%$ | $50.23 \%$ | $53.59 \%$ |
|  | MIp | $16.33 \%$ | $17.25 \%$ | $18.40 \%$ | $18.35 \%$ |
|  | MIp+ND | $33.86 \%$ | $35.45 \%$ | $37.81 \%$ | $41.74 \%$ |
|  | MIp+BND | $38.73 \%$ | $40.56 \%$ | $43.20 \%$ | $46.42 \%$ |
|  | MIp | $12.42 \%$ | $13.10 \%$ | $14.03 \%$ | $15.14 \%$ |
| Top $L$ | MIp+ND | $24.35 \%$ | $25.82 \%$ | $27.89 \%$ | $30.66 \%$ |
|  | MIp+BND | $28.11 \%$ | $29.75 \%$ | $32.16 \%$ | $35.26 \%$ |

Part 3 DCA

| Evaluation <br> methods | Predictors | $\|\mathbf{i - j}\|>\mathbf{2 3}$ | $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 0}$ | $\|\mathbf{i - j}\|>\mathbf{1 5}$ | $\|\mathbf{i - j} \mathbf{j}\|>\mathbf{8}$ |
| :---: | :--- | :--- | :--- | :--- | :--- |
| Top $L / 10$ | DCA | $54.92 \%$ | $55.81 \%$ | $57.94 \%$ | $60.26 \%$ |
|  | DCA+ND | $56.06 \%$ | $57.27 \%$ | $60.27 \%$ | $63.70 \%$ |
|  | DCA+BND | $58.03 \%$ | $58.85 \%$ | $62.01 \%$ | $65.54 \%$ |


| Top $L / 5$ | DCA | $50.55 \%$ | $51.54 \%$ | $53.84 \%$ | $57.02 \%$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | DCA+ND | $51.42 \%$ | $52.83 \%$ | $55.09 \%$ | $58.14 \%$ |
|  | DCA+BND | $53.44 \%$ | $54.51 \%$ | $56.92 \%$ | $60.46 \%$ |
|  | DCA | $40.00 \%$ | $41.68 \%$ | $44.33 \%$ | $47.53 \%$ |
| Top $L / 2$ | DCA+ND | $40.81 \%$ | $42.77 \%$ | $45.55 \%$ | $49.02 \%$ |
|  | DCA+BND | $42.39 \%$ | $44.34 \%$ | $47.18 \%$ | $50.51 \%$ |
|  | DCA | $29.18 \%$ | $30.81 \%$ | $33.56 \%$ | $37.24 \%$ |
|  | DCA+ND | $29.58 \%$ | $31.36 \%$ | $34.18 \%$ | $37.93 \%$ |
|  | DCA+BND | $30.72 \%$ | $32.74 \%$ | $35.52 \%$ | $39.48 \%$ |

## Part 4 PSICOV

| Evaluation methods | Predictors | $\|i-j\|>23$ | \|i-j|>20 | $\|i-j\|>15$ | $\|i-j\|>8$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | PSICOV | 71.77\% | 72.84\% | 74.96\% | 76.88\% |
|  | PSICOV+ND | 70.53\% | 71.95\% | 74.27\% | 77.08\% |
|  | PSICOV+BND | 71.22\% | 72.37\% | 74.51\% | 77.01\% |
| Top L/5 | PSICOV | 62.56\% | 64.21\% | 67.01\% | 70.59\% |
|  | PSICOV+ND | 60.69\% | 62.57\% | 65.85\% | 69.56\% |
|  | PSICOV+BND | 62.42\% | 63.77\% | 66.81\% | 70.29\% |
| Top L/2 | PSICOV | 44.74\% | 46.99\% | 50.02\% | 54.79\% |
|  | PSICOV+ND | 42.10\% | 44.58\% | 47.92\% | 52.85\% |
|  | PSICOV+BND | 44.05\% | 46.26\% | 49.83\% | 54.82\% |
| Top $L$ | PSICOV | 31.48\% | 33.43\% | 36.22\% | 40.49\% |
|  | PSICOV+ND | 28.60\% | 30.50\% | 33.18\% | 37.65\% |
|  | PSICOV+BND | 29.91\% | 31.90\% | 34.64\% | 39.14\% |

## Part 5 gDCA

| Evaluation methods | Predictors | $\|i-j\|>23$ | $24>\|i-j\|>11$ | 12>\|i-j|>5 | $\|i-j\|>5$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Top L/10 | gDCA | 72.86\% | 73.91\% | 76.00\% | 76.67\% |
|  | gDCA+ND | 72.86\% | 73.99\% | 76.14\% | 78.80\% |
|  | gDCA+BND | 73.62\% | 74.63\% | 77.08\% | 78.80\% |
| Top L/5 | gDCA | 64.70\% | 66.27\% | 68.50\% | 71.63\% |
|  | gDCA+ND | 64.31\% | 65.55\% | 68.18\% | 72.12\% |
|  | gDCA+BND | 66.38\% | 67.62\% | 69.64\% | 73.64\% |
| Top $L / 2$ | gDCA | 50.61\% | 52.72\% | 55.81\% | 59.38\% |
|  | gDCA+ND | 47.27\% | 49.43\% | 52.82\% | 58.31\% |
|  | gDCA+BND | 50.39\% | 52.43\% | 55.96\% | 61.13\% |
| Top $L$ | gDCA | 36.90\% | 38.94\% | 41.80\% | 47.19\% |
|  | gDCA+ND | 32.24\% | 34.27\% | 37.25\% | 43.49\% |
|  | gDCA+BND | 35.19\% | 37.31\% | 40.61\% | 46.77\% |

Table S10. The $\boldsymbol{p}$-value in the $\boldsymbol{t}$-test on all contacts.

| Method | CASP9 <br> $\|\mathbf{i} \mathbf{- j}\|>5$ | CASP9 <br> $\|\mathbf{i}-\mathbf{j}\|>23$ | CASP10 <br> $\|\mathbf{i}-\mathbf{j}\|>5$ | CASP10 <br> $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ | PSICOV <br> $\|\mathbf{i}-\mathbf{j}\|>5$ | PSICOV <br> $\|\mathbf{i}-\mathbf{j}\|>\mathbf{2 3}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| MI/ND | $1.24 \mathrm{E}-05$ | $5.05 \mathrm{E}-03$ | $9.06 \mathrm{E}-04$ | $1.69 \mathrm{E}-03$ | $7.40 \mathrm{E}-14$ | $1.99 \mathrm{E}-06$ |
| MI/BND | $3.57 \mathrm{E}-03$ | $4.12 \mathrm{E}-03$ | $1.38 \mathrm{E}-03$ | $2.42 \mathrm{E}-03$ | $8.55 \mathrm{E}-14$ | $2.20 \mathrm{E}-06$ |
| ND/BND | $1.75 \mathrm{E}-03$ | $1.18 \mathrm{E}-02$ | $3.48 \mathrm{E}-03$ | $1.28 \mathrm{E}-02$ | $1.89 \mathrm{E}-05$ | $1.08 \mathrm{E}-05$ |
| MIp/ND | $5.44 \mathrm{E}-06$ | $3.01 \mathrm{E}-03$ | $9.15 \mathrm{E}-04$ | $7.28 \mathrm{E}-05$ | $7.34 \mathrm{E}-14$ | $1.99 \mathrm{E}-06$ |
| MIp/BND | $3.69 \mathrm{E}-04$ | $5.01 \mathrm{E}-03$ | $1.40 \mathrm{E}-03$ | $7.17 \mathrm{E}-04$ | $8.35 \mathrm{E}-14$ | $2.17 \mathrm{E}-06$ |
| ND/BND | $3.18 \mathrm{E}-04$ | $6.95 \mathrm{E}-03$ | $1.36 \mathrm{E}-02$ | $9.81 \mathrm{E}-03$ | $1.19 \mathrm{E}-03$ | $3.96 \mathrm{E}-05$ |
| DCA/ND | $1.00 \mathrm{E}-07$ | $4.54 \mathrm{E}-05$ | $3.55 \mathrm{E}-05$ | $3.54 \mathrm{E}-06$ | $7.55 \mathrm{E}-14$ | $2.08 \mathrm{E}-06$ |
| DCA/BND | $1.99 \mathrm{E}-07$ | $7.45 \mathrm{E}-05$ | $2.91 \mathrm{E}-04$ | $3.93 \mathrm{E}-07$ | $4.79 \mathrm{E}-13$ | $8.29 \mathrm{E}-06$ |
| ND/BND | $9.73 \mathrm{E}-04$ | $3.12 \mathrm{E}-03$ | $2.83 \mathrm{E}-04$ | $3.32 \mathrm{E}-04$ | $5.66 \mathrm{E}-13$ | $1.08 \mathrm{E}-05$ |
| PSICOV/ND | $2.32 \mathrm{E}-09$ | $3.27 \mathrm{E}-06$ | $8.11 \mathrm{E}-06$ | $8.11 \mathrm{E}-06$ | $5.78 \mathrm{E}-13$ | $5.30 \mathrm{E}-06$ |
| PSICOV/BND | $2.16 \mathrm{E}-07$ | $1.00 \mathrm{E}-05$ | $4.25 \mathrm{E}-06$ | $4.25 \mathrm{E}-06$ | $2.63 \mathrm{E}-13$ | $3.83 \mathrm{E}-06$ |
| ND/BND | $6.72 \mathrm{E}-08$ | $2.12 \mathrm{E}-04$ | $8.80 \mathrm{E}-05$ | $8.80 \mathrm{E}-05$ | $1.70 \mathrm{E}-11$ | $5.95 \mathrm{E}-05$ |
| gDCA/ND | $4.13 \mathrm{E}-04$ | $3.01 \mathrm{E}-03$ | $7.19 \mathrm{E}-03$ | $8.75 \mathrm{E}-03$ | $1.23 \mathrm{E}-02$ | $1.06 \mathrm{E}-02$ |
| gDCA/BND | $2.78 \mathrm{E}-03$ | $9.87 \mathrm{E}-03$ | $1.43 \mathrm{E}-02$ | $2.50 \mathrm{E}-02$ | $6.48 \mathrm{E}-02$ | $4.80 \mathrm{E}-02$ |
| ND/BND | $3.30 \mathrm{E}-02$ | $2.20 \mathrm{E}-02$ | $5.55 \mathrm{E}-03$ | $1.48 \mathrm{E}-02$ | $4.78 \mathrm{E}-03$ | $6.41 \mathrm{E}-03$ |

