Supplementary information

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CONTENTS

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

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

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

Part 1 MI

Part 2 MIp

Evaluation	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
methods	<u> </u>		1.01	1 91 	1 91
	MIp	10.39%	8.79%	9.57%	11.74%
Top <i>L</i> /10	MIp+ND	22.22%	17.73%	18.23%	25.30%
	MIp+BND	26.49%	21.93%	21.11%	30.46%
	MIp	8.46%	7.37%	8.49%	10.26%
Top <i>L</i> /5	MIp+ND	18.13%	14.39%	15.32%	22.15%
	MIp+BND	21.26%	17.43%	16.55%	26.57%
	MIp	6.16%	6.41%	7.65%	8.31%
Top <i>L</i> /2	MIp+ND	13.19%	10.72%	11.60%	16.94%
	MIp+BND	15.81%	12.52%	12.52%	19.86%
	MIp	5.19%	5.38%	6.95%	7.01%
Top L	MIp+ND	10.25%	8.28%	9.21%	13.34%
	MIp+BND	12.38%	9.71%	10.09%	15.72%
		Part	t 3 DCA		
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	DCA	29.88%	24.76%	20.33%	31.89%
Top <i>L</i> /10	DCA+ND	29.86%	24.51%	22.72%	32.81%
1	DCA+BND	31.34%	25.68%	23.57%	35.00%

Top <i>L</i> /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%
Top <i>L</i> /2	DCA	17.69%	12.65%	12.70%	21.58%
	DCA+ND	17.82%	13.07%	13.33%	22.76%
	DCA+BND	18.87%	14.05%	14.28%	23.96%
Top L	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
-	PSICOV	31.94%	23.33%	22.14%	36.18%
Top <i>L</i> /10	PSICOV+ND	31.57%	22.26%	22.39%	36.22%
	PSICOV+BND	33.70%	24.70%	24.92%	40.07%
	PSICOV	25.02%	17.88%	17.70%	29.41%
Top <i>L</i> /5	PSICOV+ND	24.47%	17.16%	17.29%	30.46%
	PSICOV+BND	26.21%	18.89%	18.97%	33.24%
	PSICOV	17.53%	12.64%	13.09%	21.80%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	gDCA	34.29%	25.98%	21.50%	36.36%
Top <i>L</i> /10	gDCA+ND	35.32%	25.87%	20.89%	34.91%
	gDCA+BND	35.87%	27.06%	22.27%	38.05%
	gDCA	27.66%	20.75%	18.96%	31.18%
Top <i>L</i> /5	gDCA+ND	28.57%	20.39%	17.64%	30.30%
	gDCA+BND	29.06%	20.87%	18.17%	32.56%
	gDCA	20.71%	14.55%	14.32%	23.59%
Top <i>L</i> /2	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.

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

Part 1 MI

Part 2 MIp

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5	
	MIp	15.82%	17.42%	14.06%	19.36%	
Top <i>L</i> /10	MIp+ND	30.81%	33.23%	24.92%	38.70%	
	MIp+BND	36.53%	36.69%	28.29%	42.83%	
	MIp	13.82%	13.40%	11.90%	16.31%	
Top <i>L</i> /5	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%	
Top <i>L</i> /2	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 methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5	
	DCA	40.74%	39.56%	29.50%	44.06%	
Top <i>L</i> /10	DCA+ND	38.98%	39.10%	32.00%	46.07%	
	DCA+BND	41.42%	40.04%	33.80%	48.94%	

Top <i>L</i> /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%
Top <i>L</i> /2	DCA	25.94%	22.81%	16.73%	33.00%
	DCA+ND	25.96%	23.11%	17.16%	34.73%
	DCA+BND	26.80%	24.02%	17.74%	36.14%
Top L	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%

Evaluation methods	Predictors	i - j >23	24> i-j >11	12> i-j >5	i-j >5
	PSICOV	41.45%	41.61%	31.57%	51.58%
Top <i>L</i> /10	PSICOV+ND	39.89%	40.73%	30.80%	50.56%
	PSICOV+BND	41.55%	40.66%	33.48%	51.48%
	PSICOV	35.87%	32.63%	24.69%	44.82%
Top <i>L</i> /5	PSICOV+ND	34.75%	31.33%	23.84%	44.48%
	PSICOV+BND	36.50%	32.28%	24.96%	46.47%
	PSICOV	26.72%	22.55%	17.04%	35.57%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	gDCA	45.22%	44.61%	34.05%	51.56%
Top <i>L</i> /10	gDCA+ND	42.78%	42.89%	33.51%	51.43%
	gDCA+BND	45.13%	44.14%	35.42%	52.72%
	gDCA	40.11%	36.95%	27.29%	47.07%
Top <i>L</i> /5	gDCA+ND	38.26%	34.30%	27.00%	47.32%
	gDCA+BND	39.67%	36.23%	27.70%	48.54%
	gDCA	30.36%	25.53%	18.60%	39.19%
Top <i>L</i> /2	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%

	Part 1 MI						
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5		
	MI	7.62%	5.46%	7.32%	10.08%		
Top <i>L</i> /10	MI+ND	14.47%	13.07%	13.99%	18.37%		
	MI+BND	20.53%	18.13%	19.20%	27.02%		
	MI	6.59%	4.45%	6.62%	8.17%		
Top <i>L</i> /5	MI+ND	13.04%	9.25%	12.37%	15.27%		
	MI+BND	16.41%	13.31%	14.54%	23.25%		
	MI	4.81%	4.51%	6.14%	5.72%		
Top <i>L</i> /2	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%		

in CASP9 dataset.

Part 2 MIp

			1			
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5	
	MIp	7.62%	5.46%	7.32%	10.25%	
Top <i>L</i> /10	MIp+ND	15.38%	12.26%	15.37%	18.63%	
	MIp+BND	20.88%	17.66%	20.01%	26.77%	
	MIp	6.59%	4.45%	6.62%	8.17%	
Top <i>L</i> /5	MIp+ND	13.33%	9.29%	13.16%	15.22%	
	MIp+BND	15.75%	13.67%	14.83%	22.76%	
	MIp	4.81%	4.56%	6.22%	5.72%	
Top <i>L</i> /2	MIp+ND	9.93%	7.54%	10.22%	12.27%	
	MIp+BND	12.14%	9.65%	10.85%	16.49%	
	MIp	4.04%	4.43%	6.15%	5.10%	
Top L	MIp+ND	7.44%	6.39%	7.94%	10.00%	
	MIp+BND	9.23%	7.91%	8.74%	12.68%	
Part 3 DCA						
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i -j >5	
	DCA	25.61%	17.61%	19.23%	28.14%	
Top <i>L</i> /10	DCA+ND	26.04%	16.79%	21.49%	27.49%	
	DCA+BND	24.56%	16.58%	21.32%	27.51%	

Top <i>L</i> /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%
Top <i>L</i> /2	DCA+ND	12.60%	9.16%	10.55%	17.49%
1	DCA+BND	13.26%	10.24%	11.91%	18.60%
Top L	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	PSICOV	23.43%	17.73%	18.14%	29.78%
Top <i>L</i> /10	PSICOV+ND	22.63%	16.54%	17.68%	29.00%
	PSICOV+BND	24.44%	17.33%	18.14%	30.63%
	PSICOV	17.35%	13.86%	14.14%	22.95%
Top <i>L</i> /5	PSICOV+ND	16.61%	12.53%	13.15%	22.44%
	PSICOV+BND	17.19%	12.85%	13.79%	24.25%
	PSICOV	12.72%	9.47%	10.95%	15.79%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	gDCA	29.30%	20.52%	18.57%	31.13%
Top <i>L</i> /10	gDCA+ND	29.55%	16.61%	17.68%	29.02%
	gDCA+BND	29.53%	18.99%	18.91%	32.01%
	gDCA	21.75%	15.75%	16.54%	26.98%
Top <i>L</i> /5	gDCA+ND	22.11%	13.74%	15.72%	24.63%
	gDCA+BND	21.84%	14.79%	15.33%	25.81%
	gDCA	15.16%	11.10%	11.68%	19.22%
Top <i>L</i> /2	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%

Part 1 MI							
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5		
-	MI	9.48%	12.60%	7.71%	10.88%		
Top <i>L</i> /10	MI+ND	13.89%	21.72%	13.35%	19.99%		
	MI+BND	18.61%	23.47%	17.55%	24.09%		
	MI	8.27%	9.78%	7.05%	8.83%		
Top <i>L</i> /5	MI+ND	12.04%	17.81%	10.48%	16.84%		
	MI+BND	15.72%	19.66%	13.21%	20.91%		
	MI	6.54%	6.98%	6.34%	7.33%		
Top <i>L</i> /2	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%		

in CASP10 dataset.

Part 2 MIp

Evaluation					
methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	MIp	9.48%	12.60%	7.71%	10.88%
Top <i>L</i> /10	MIp+ND	13.99%	21.26%	13.66%	20.70%
	MIp+BND	17.83%	22.62%	17.16%	24.09%
	MIp	8.27%	10.18%	7.05%	9.33%
Top <i>L</i> /5	MIp+ND	12.04%	18.10%	11.08%	17.08%
	MIp+BND	16.59%	19.89%	13.47%	20.51%
	MIp	6.70%	6.93%	7.28%	7.36%
Top <i>L</i> /2	MIp+ND	9.61%	12.79%	9.03%	13.20%
	MIp+BND	11.76%	14.87%	10.71%	15.41%
	MIp	5.30%	5.70%	6.22%	6.40%
Top L	MIp+ND	7.32%	10.57%	7.71%	10.55%
	MIp+BND	9.22%	12.00%	8.56%	12.44%
		_			
		Par	t 3 DCA		
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	DCA	19.08%	22.89%	17.09%	22.94%
Top <i>L</i> /10	DCA+ND	16.61%	21.07%	17.25%	24.28%
	DCA+BND	20.30%	23.74%	18.71%	28.53%

Top <i>L</i> /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 <i>L</i> /2	DCA+ND	11.13%	15.58%	10.45%	17.51%
	DCA+BND	11.74%	16.19%	10.87%	18.72%
Top L	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%

Evaluation methods	Predictors	i - j >23	24> i-j >11	12> i-j >5	i-j >5
-	PSICOV	17.58%	24.89%	15.62%	27.20%
Top <i>L</i> /10	PSICOV+ND	16.10%	24.12%	13.96%	27.49%
	PSICOV+BND	19.09%	23.33%	15.82%	29.83%
	PSICOV	15.39%	18.77%	11.14%	21.90%
Top <i>L</i> /5	PSICOV+ND	14.11%	18.68%	11.45%	22.24%
	PSICOV+BND	16.10%	18.81%	11.60%	24.37%
	PSICOV	11.34%	14.65%	9.74%	16.89%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	gDCA	20.86%	27.05%	17.10%	27.90%
Top <i>L</i> /10	gDCA+ND	19.28%	22.49%	16.23%	27.39%
	gDCA+BND	21.82%	25.23%	16.80%	28.65%
	gDCA	18.04%	21.73%	14.69%	23.79%
Top <i>L</i> /5	gDCA+ND	16.56%	19.99%	14.00%	24.35%
	gDCA+BND	17.66%	21.35%	12.98%	25.67%
	gDCA	13.31%	16.74%	10.73%	19.11%
Top <i>L</i> /2	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 **Predictors** |**i**-**j**|>23 24>|i-j|>11 12>|i-j|>5 |i-j|>5 methods MI 30.28% 29.12% 22.26% 19.83% Top *L*/10 MI+ND 55.04% 45.59% 39.74% 61.93% MI+BND 60.76% 50.03% 43.11% 66.36% MI 23.15% 16.95% 16.17% 25.08%35.47% Top *L*/5 MI+ND 46.89% 30.37% 53.90% MI+BND 39.96% 33.28% 58.84% 52.23% MI 18.71% 16.33% 12.39% 11.94% Top *L*/2 MI+ND 33.58% 22.41% 19.70% 42.11% MI+BND 38.61% 25.77% 21.34% 46.19% 15.50% MI 12.42% 9.32% 9.84% Top LMI+ND 24.18%15.15% 13.81% 31.83% MI+BND 27.99% 35.57% 17.19% 14.81%

Part 2 MIp

		- ***	·P					
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5			
	MIp	29.12%	22.26%	19.83%	30.28%			
Top <i>L</i> /10	MIp+ND	55.15%	45.68%	39.66%	62.07%			
	MIp+BND	60.20%	50.12%	43.29%	65.83%			
	MIp	23.15%	16.95%	16.17%	25.08%			
Top <i>L</i> /5	MIp+ND	46.96%	35.53%	30.60%	53.96%			
	MIp+BND	52.29%	40.03%	33.26%	58.87%			
	MIp	16.33%	12.39%	11.94%	18.71%			
Top <i>L</i> /2	MIp+ND	33.86%	22.60%	19.94%	42.21%			
	MIp+BND	38.73%	25.96%	21.57%	46.11%			
	MIp	12.42%	9.32%	9.84%	15.50%			
Top L	MIp+ND	24.35%	15.36%	13.88%	31.90%			
	MIp+BND	28.11%	17.25%	14.92%	35.59%			
Part 3 DCA								
Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5			
	DCA	54.92%	53.45%	43.33%	60.14%			
Top <i>L</i> /10	DCA+ND	56.06%	54.89%	46.37%	63.57%			
*	DCA+BND	58.03%	56.86%	48.73%	65.96%			

Top <i>L</i> /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 <i>L</i> /2	DCA+ND	40.81%	27.04%	22.61%	49.92%
	DCA+BND	42.39%	28.24%	23.34%	51.66%
Top L	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%

Evaluation methods	Predictors	i - j >23	24> i-j >11	12> i-j >5	i-j >5
	PSICOV	71.77%	58.11%	50.95%	77.11%
Top <i>L</i> /10	PSICOV+ND	70.53%	56.97%	49.72%	76.66%
	PSICOV+BND	71.22%	57.60%	51.25%	77.03%
	PSICOV	62.56%	45.87%	38.62%	71.19%
Top <i>L</i> /5	PSICOV+ND	60.69%	43.27%	36.77%	70.28%
	PSICOV+BND	62.42%	44.82%	38.06%	70.65%
	PSICOV	44.74%	27.81%	23.94%	56.22%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
-	gDCA	72.86%	60.79%	54.59%	76.56%
Top <i>L</i> /10	gDCA+ND	72.86%	61.51%	54.04%	78.73%
	gDCA+BND	73.62%	62.96%	56.63%	78.52%
	gDCA	64.70%	50.28%	42.15%	71.81%
Top <i>L</i> /5	gDCA+ND	64.31%	47.48%	40.33%	72.11%
	gDCA+BND	66.38%	50.16%	42.44%	73.86%
	gDCA	50.61%	31.81%	26.32%	59.94%
Top <i>L</i> /2	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

Part 1 MI								
Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8			
-	MI	10.39%	10.68%	10.68%	11.59%			
Top <i>L</i> /10	MI+ND	21.60%	22.26%	23.28%	25.19%			
	MI+BND	26.29%	27.66%	28.81%	31.44%			
	MI	8.41%	8.58%	9.09%	10.03%			
Top <i>L</i> /5	MI+ND	17.73%	18.68%	19.65%	21.50%			
	MI+BND	21.58%	22.40%	23.49%	26.34%			
	MI	6.12%	6.51%	6.98%	7.58%			
Top <i>L</i> /2	MI+ND	12.95%	13.43%	14.22%	16.16%			
	MI+BND	15.49%	16.38%	17.36%	19.37%			
	MI	5.16%	5.43%	5.82%	6.47%			
Top L	MI+ND	10.05%	10.52%	11.31%	12.47%			
	MI+BND	11.86%	12.55%	13.39%	14.90%			

dataset at different cutoff values of long-range contacts.

Part 2 MIp

Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8
-	MIp	10.39%	10.68%	10.68%	11.37%
Top <i>L</i> /10	MIp+ND	22.22%	22.64%	23.56%	25.28%
	MIp+BND	26.49%	27.24%	28.80%	30.40%
	MIp	8.46%	8.66%	9.06%	9.94%
Top <i>L</i> /5	MIp+ND	18.13%	18.79%	19.82%	21.64%
	MIp+BND	21.26%	22.74%	23.36%	25.75%
	MIp	6.16%	6.54%	6.95%	7.60%
Top <i>L</i> /2	MIp+ND	13.19%	13.80%	14.59%	16.23%
	MIp+BND	15.81%	16.50%	17.50%	19.45%
	MIp	5.19%	5.44%	5.82%	6.44%
Top L	MIp+ND	10.25%	10.76%	11.43%	12.58%
	MIp+BND	12.38%	12.96%	13.79%	14.99%
		Part	3 DCA		
Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8
	DCA	29.88%	30.49%	31.21%	33.19%
Top <i>L</i> /10	DCA+ND	29.86%	30.51%	31.80%	33.90%
	DCA+BND	31.34%	31.42%	32.89%	35.67%

Top <i>L</i> /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%
Top <i>L</i> /2	DCA+ND	17.82%	18.78%	20.13%	22.14%
	DCA+BND	18.87%	19.75%	21.30%	23.24%
Top L	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%

Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8
	PSICOV	31.94%	32.21%	33.90%	36.73%
Top <i>L</i> /10	PSICOV+ND	31.57%	31.99%	33.32%	36.70%
	PSICOV+BND	33.70%	34.23%	35.89%	39.54%
	PSICOV	25.02%	26.28%	27.16%	29.76%
Top <i>L</i> /5	PSICOV+ND	24.47%	25.52%	26.88%	29.93%
	PSICOV+BND	26.21%	27.58%	28.94%	32.62%
	PSICOV	17.53%	18.56%	19.27%	20.97%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
-	gDCA	34.29%	35.67%	36.55%	38.02%
Top <i>L</i> /10	gDCA+ND	35.32%	35.67%	36.32%	37.44%
	gDCA+BND	35.87%	36.57%	37.37%	39.63%
	gDCA	27.66%	28.95%	29.73%	32.23%
Top <i>L</i> /5	gDCA+ND	28.57%	29.68%	30.84%	32.18%
	gDCA+BND	29.06%	30.17%	31.25%	33.90%
	gDCA	20.71%	21.43%	21.99%	23.65%
Top <i>L</i> /2	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

Part 1 MI							
Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8		
	MI	15.82%	18.81%	17.77%	19.77%		
Top <i>L</i> /10	MI+ND	30.63%	35.39%	36.62%	40.60%		
	MI+BND	36.78%	39.65%	40.66%	44.97%		
	MI	13.82%	16.30%	14.70%	16.78%		
Top <i>L</i> /5	MI+ND	25.45%	29.22%	30.98%	33.80%		
	MI+BND	30.77%	34.33%	36.02%	39.24%		
	MI	9.97%	11.97%	11.68%	12.69%		
Top <i>L</i> /2	MI+ND	18.89%	21.93%	23.71%	26.14%		
	MI+BND	22.63%	26.04%	27.79%	30.48%		
	MI	7.71%	9.67%	9.47%	9.84%		
Top L	MI+ND	14.15%	17.05%	18.31%	20.03%		
	MI+BND	16.69%	19.61%	21.25%	23.36%		

dataset at different cutoff values of long-range contacts.

Part 2 MIp

		Iuitz	amp					
Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8			
	MIp	15.82%	18.81%	17.77%	19.86%			
Top <i>L</i> /10	MIp+ND	30.81%	35.52%	37.01%	40.45%			
	MIp+BND	36.53%	39.63%	40.81%	45.05%			
	MIp	13.82%	16.30%	14.82%	16.99%			
Top <i>L</i> /5	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%			
Top <i>L</i> /2	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 methods	Predictors	i - j >23	i-j >20	i-j >15	i-j >8			
	DCA	40.74%	44.21%	44.66%	46.96%			
Top <i>L</i> /10	DCA+ND	38.98%	42.98%	44.49%	47.13%			
	DCA+BND	41.42%	45.41%	46.73%	49.49%			

Top <i>L</i> /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 <i>L</i> /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%
Top L	DCA+ND	18.79%	22.55%	24.59%	27.27%
	DCA+BND	19.51%	23.30%	25.55%	28.24%

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

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
	gDCA	45.22%	47.87%	49.55%	51.77%
Top <i>L</i> /10	gDCA+ND	42.78%	46.16%	47.82%	50.89%
	gDCA+BND	45.13%	47.99%	48.89%	51.87%
	gDCA	40.11%	44.07%	45.97%	47.68%
Top <i>L</i> /5	gDCA+ND	38.26%	42.79%	44.02%	46.96%
	gDCA+BND	39.67%	44.08%	46.07%	48.32%
	gDCA	30.36%	34.74%	37.07%	39.32%
Top <i>L</i> /2	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

Part 1 MI							
Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8		
-	MI	29.12%	29.91%	32.40%	31.83%		
Top <i>L</i> /10	MI+ND	55.04%	55.65%	58.04%	61.57%		
	MI+BND	60.76%	61.32%	64.08%	67.30%		
	MI	23.15%	23.54%	24.73%	25.79%		
Top <i>L</i> /5	MI+ND	46.89%	47.76%	50.19%	53.64%		
	MI+BND	52.23%	53.87%	56.63%	59.45%		
	MI	16.33%	17.25%	18.40%	18.91%		
Top <i>L</i> /2	MI+ND	33.58%	35.30%	37.59%	41.55%		
	MI+BND	38.61%	40.46%	43.21%	46.32%		
	MI	12.42%	13.10%	14.03%	15.14%		
Top L	MI+ND	24.18%	25.73%	27.72%	30.57%		
	MI+BND	27.99%	29.72%	31.95%	35.09%		

dataset at different cutoff values of long-range contacts.

Part 2 MIp

		I ult 2	2 mil					
Evaluation methods	Predictors	i - j >23	i-j >20	i-j >15	i-j >8			
	MIp	29.12%	29.91%	32.40%	31.83%			
Top <i>L</i> /10	MIp+ND	55.15%	55.89%	58.28%	61.69%			
	MIp+BND	60.20%	61.02%	63.79%	66.99%			
	MIp	23.15%	23.54%	24.73%	25.79%			
Top <i>L</i> /5	MIp+ND	46.96%	47.96%	50.23%	53.59%			
	MIp+BND	52.29%	53.94%	56.73%	59.35%			
	MIp	16.33%	17.25%	18.40%	18.91%			
Top <i>L</i> /2	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 methods	Predictors	i - j >23	i-j >20	i-j >15	i-j >8			
	DCA	54.92%	55.81%	57.94%	60.26%			
Top <i>L</i> /10	DCA+ND	56.06%	57.27%	60.27%	63.70%			
	DCA+BND	58.03%	58.85%	62.01%	65.54%			

Top <i>L</i> /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%
Top <i>L</i> /2	DCA	40.00%	41.68%	44.33%	47.53%
	DCA+ND	40.81%	42.77%	45.55%	49.02%
	DCA+BND	42.39%	44.34%	47.18%	50.51%
Top L	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%

Evaluation methods	Predictors	i-j >23	i-j >20	i-j >15	i-j >8
Top <i>L</i> /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%
	PSICOV	62.56%	64.21%	67.01%	70.59%
Top <i>L</i> /5	PSICOV+ND	60.69%	62.57%	65.85%	69.56%
	PSICOV+BND	62.42%	63.77%	66.81%	70.29%
	PSICOV	44.74%	46.99%	50.02%	54.79%
Top <i>L</i> /2	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%

Evaluation methods	Predictors	i-j >23	24> i-j >11	12> i-j >5	i-j >5
Top <i>L</i> /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 <i>L</i> /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 <i>L</i> /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%

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

 Table S10. The *p*-value in the *t*-test on all contacts.