

Supplementary data:

Table S1: Contact preferences of residue pairs (sorted by p-values). Total number of residue pairs in the entire data set is 7,750,982 of which 11,259 have at least one contact within (one residue of the pair is less than 6.0Å from the other).

Residue Pair	# Occurrences	Propensity	Observed no. of contacting pairs	Expected no. of contacting pairs	Chi-square	p-value
D-R	38053	2.9	161	55.3	202.2	6.85E-46
R-Y	27214	3.0	119	39.5	159.8	1.28E-36
N-Y	27275	3.0	118	39.6	155.1	1.36E-35
E-R	43020	2.4	152	62.5	128.2	1.01E-29
R-W	10880	3.6	57	15.8	107.4	3.67E-25
N-R	29478	2.4	104	42.8	87.4	8.80E-21
K-Y	38155	2.2	124	55.4	84.9	3.22E-20
D-K	53701	2.0	158	78.0	82.0	1.34E-19
E-K	61956	1.9	172	90.0	74.7	5.42E-18
W-Y	10501	3.2	49	15.3	74.7	5.60E-18
T-Y	40180	2.1	124	58.4	73.8	8.60E-18
Q-Y	24241	2.4	85	35.2	70.4	4.85E-17
D-Y	33431	2.1	101	48.6	56.6	5.27E-14
F-Y	23691	2.3	78	34.4	55.2	1.09E-13
Q-R	26173	2.2	83	38.0	53.2	2.98E-13
A-V	74917	0.3	34	108.8	51.4	7.36E-13
P-Y	29237	2.0	85	42.5	42.6	6.74E-11

M-Y	12988	2.5	47	18.9	42.0	9.35E-11
G-Y	43696	1.8	115	63.5	41.8	9.95E-11
N-Q	26939	2.0	79	39.1	40.6	1.85E-10
A-L	90550	0.5	60	131.5	38.9	4.46E-10
L-V	94746	0.5	65	137.6	38.3	5.99E-10
K-V	69074	0.4	40	100.3	36.3	1.71E-09
H-R	13625	2.3	46	19.8	34.7	3.83E-09
H-Y	12473	2.4	43	18.1	34.2	5.05E-09
E-L	84917	0.5	59	123.3	33.6	6.87E-09
E-V	70674	0.4	45	102.7	32.4	1.26E-08
I-V	57344	0.4	32	83.3	31.6	1.90E-08
A-P	49550	0.3	25	72.0	30.7	3.08E-08
P-W	12271	2.3	41	17.8	30.1	4.04E-08
D-L	74253	0.5	51	107.9	30.0	4.38E-08
S-Y	45371	1.7	110	65.9	29.5	5.59E-08
S-V	81876	0.5	61	118.9	28.2	1.08E-07
A-E	67785	0.5	46	98.5	28.0	1.24E-07
A-D	58846	0.5	39	85.5	25.3	4.98E-07
N-T	44581	1.6	105	64.8	25.0	5.71E-07
P-V	50955	0.4	31	74.0	25.0	5.73E-07
A-K	66873	0.5	49	97.1	23.9	1.04E-06
Q-W	9977	2.3	33	14.5	23.6	1.16E-06
A-S	78135	0.5	62	113.5	23.4	1.34E-06

L-S	99102	0.6	86	144.0	23.3	1.36E-06
A-A	35784	0.3	18	52.0	22.2	2.44E-06
D-N	37447	1.6	89	54.4	22.0	2.71E-06
I-T	51263	0.5	34	74.5	22.0	2.74E-06
T-V	71896	0.5	57	104.4	21.5	3.46E-06
R-R	14846	2.0	43	21.6	21.3	3.92E-06
H-W	4767	2.7	19	6.9	21.1	4.46E-06
C-T	21962	0.2	6	31.9	21.0	4.52E-06
A-I	55011	0.5	40	79.9	19.9	8.03E-06
G-W	18160	1.9	49	26.4	19.4	1.06E-05
E-Y	39234	1.6	90	57.0	19.1	1.23E-05
A-G	75458	0.6	64	109.6	19.0	1.32E-05
K-L	84632	0.6	75	122.9	18.7	1.54E-05
R-T	44625	1.5	99	64.8	18.0	2.18E-05
L-Y	53527	1.5	115	77.8	17.8	2.40E-05
T-W	17879	1.8	47	26.0	17.0	3.68E-05
E-I	51844	0.5	40	75.3	16.6	4.73E-05
I-Y	30846	1.6	72	44.8	16.5	4.86E-05
D-Q	33025	1.6	76	48.0	16.4	5.19E-05
G-L	92001	0.7	88	133.6	15.6	7.88E-05
G-V	79029	0.6	74	114.8	14.5	1.40E-04
L-T	87113	0.7	84	126.5	14.3	1.56E-04
D-V	61006	0.6	54	88.6	13.5	2.36E-04

E-N	42843	1.5	91	62.2	13.3	2.66E-04
V-V	39454	0.5	30	57.3	13.0	3.09E-04
L-P	61194	0.6	55	88.9	12.9	3.25E-04
N-N	14801	1.8	38	21.5	12.7	3.73E-04
N-W	11394	1.9	31	16.6	12.6	3.83E-04
A-T	69472	0.7	66	100.9	12.1	5.10E-04
F-V	42113	0.6	34	61.2	12.1	5.12E-04
C-E	20611	0.4	11	29.9	12.0	5.38E-04
G-P	51288	0.6	45	74.5	11.7	6.31E-04
G-R	48265	1.4	98	70.1	11.1	8.65E-04
R-S	51783	1.4	104	75.2	11.0	9.05E-04
A-C	22512	0.4	14	32.7	10.7	1.07E-03
W-W	2238	2.8	9	3.3	10.2	1.43E-03
F-R	26363	1.5	58	38.3	10.1	1.45E-03
H-H	3036	2.5	11	4.4	9.8	1.70E-03
A-F	40595	0.6	35	59.0	9.7	1.80E-03
C-V	23556	0.5	16	34.2	9.7	1.84E-03
I-P	36174	0.6	30	52.5	9.7	1.87E-03
G-S	80844	0.7	84	117.4	9.5	2.03E-03
H-N	13952	1.7	34	20.3	9.3	2.28E-03
A-Q	40920	0.6	37	59.4	8.5	3.61E-03
D-W	13491	1.6	32	19.6	7.9	5.08E-03
K-W	15686	1.6	36	22.8	7.7	5.63E-03

F-M	13046	1.6	31	19.0	7.7	5.64E-03
C-D	17876	0.5	12	26.0	7.5	6.13E-03
P-R	30234	1.4	62	43.9	7.4	6.36E-03
D-I	45422	0.7	44	66.0	7.3	6.81E-03
Q-T	40265	1.4	79	58.5	7.2	7.32E-03
C-N	14703	0.4	9	21.4	7.2	7.50E-03
G-Q	42084	1.3	82	61.1	7.1	7.60E-03
I-S	57812	0.7	60	84.0	6.8	8.88E-03
E-G	69737	0.7	75	101.3	6.8	8.97E-03
E-H	19960	1.5	43	29.0	6.8	9.29E-03
I-K	50360	0.7	51	73.2	6.7	9.60E-03
C-P	15286	0.5	10	22.2	6.7	9.60E-03
K-K	29365	0.6	26	42.7	6.5	1.08E-02
A-M	23170	0.6	19	33.7	6.4	1.15E-02
L-N	57843	0.7	61	84.0	6.3	1.20E-02
Y-Y	12047	1.6	28	17.5	6.3	1.21E-02
K-M	21159	0.6	17	30.7	6.1	1.32E-02
C-M	6982	1.8	18	10.1	6.1	1.36E-02
D-P	38923	0.7	38	56.5	6.1	1.37E-02
S-W	20452	1.4	43	29.7	5.9	1.47E-02
G-N	49192	1.3	92	71.5	5.9	1.51E-02
H-I	16090	1.5	35	23.4	5.8	1.62E-02
C-R	14480	1.5	32	21.0	5.7	1.68E-02

H-M	6686	1.8	17	9.7	5.5	1.94E-02
N-S	50999	1.3	94	74.1	5.4	2.07E-02
N-V	48750	0.7	52	70.8	5.0	2.54E-02
M-V	24024	0.6	22	34.9	4.8	2.90E-02
M-S	23103	1.4	46	33.6	4.6	3.17E-02
M-W	4987	1.8	13	7.2	4.6	3.25E-02
Q-V	43304	0.7	46	62.9	4.5	3.31E-02
P-T	48789	0.7	53	70.9	4.5	3.38E-02
P-S	55822	0.8	62	81.1	4.5	3.40E-02
L-W	21473	1.4	43	31.2	4.5	3.45E-02
F-Q	23442	1.4	46	34.1	4.2	4.06E-02
E-W	15520	1.4	32	22.5	4.0	4.64E-02
F-G	41615	0.7	45	60.4	3.9	4.69E-02
V-Y	43763	1.2	79	63.6	3.7	5.30E-02
I-W	12404	1.4	26	18.0	3.5	6.00E-02
A-N	45622	0.8	51	66.3	3.5	6.07E-02
E-Q	37539	1.2	68	54.5	3.3	6.81E-02
L-M	28451	1.3	53	41.3	3.3	6.94E-02
M-R	14975	1.4	30	21.8	3.1	7.70E-02
F-S	42429	0.8	48	61.6	3.0	8.25E-02
I-M	18139	0.7	18	26.3	2.6	1.04E-01
D-H	17749	1.3	34	25.8	2.6	1.06E-01
G-I	56920	0.8	68	82.7	2.6	1.06E-01

K-T	63588	0.8	77	92.4	2.6	1.10E-01
K-N	42560	1.2	74	61.8	2.4	1.21E-01
A-H	21795	0.7	23	31.7	2.4	1.24E-01
D-E	55562	0.8	67	80.7	2.3	1.27E-01
E-E	31135	0.8	35	45.2	2.3	1.28E-01
F-H	12163	1.4	24	17.7	2.3	1.32E-01
C-C	3803	0.4	2	5.5	2.2	1.34E-01
N-P	32199	1.2	57	46.8	2.2	1.35E-01
C-K	20752	0.7	22	30.1	2.2	1.38E-01
A-Y	42263	1.2	73	61.4	2.2	1.38E-01
K-P	44693	0.8	53	64.9	2.2	1.39E-01
P-Q	28573	1.2	51	41.5	2.2	1.41E-01
H-Q	12310	1.3	24	17.9	2.1	1.48E-01
G-K	69084	0.9	86	100.4	2.1	1.52E-01
Q-S	46310	1.2	79	67.3	2.0	1.53E-01
D-T	54596	1.2	92	79.3	2.0	1.54E-01
I-Q	30732	1.2	54	44.6	2.0	1.61E-01
H-V	22703	0.8	25	33.0	1.9	1.65E-01
L-R	58812	0.9	73	85.4	1.8	1.79E-01
C-L	27841	0.8	32	40.4	1.8	1.84E-01
E-T	64381	1.1	106	93.5	1.7	1.97E-01
H-S	23095	1.2	41	33.5	1.7	1.98E-01
F-F	11000	1.3	21	16.0	1.6	2.09E-01

G-M	24633	1.2	43	35.8	1.5	2.28E-01
H-L	27197	1.2	47	39.5	1.4	2.33E-01
E-M	21759	1.2	38	31.6	1.3	2.55E-01
E-P	44852	0.9	56	65.2	1.3	2.57E-01
F-P	26821	1.2	46	39.0	1.3	2.59E-01
K-S	73486	1.1	118	106.7	1.2	2.76E-01
D-G	60703	0.9	78	88.2	1.2	2.78E-01
P-P	16735	0.8	19	24.3	1.2	2.82E-01
M-N	14303	0.8	16	20.8	1.1	2.95E-01
E-F	38692	1.1	64	56.2	1.1	2.98E-01
D-F	32970	0.9	41	47.9	1.0	3.19E-01
L-L	57814	0.9	75	84.0	1.0	3.27E-01
S-T	76621	0.9	101	111.3	1.0	3.29E-01
C-Q	13200	0.8	15	19.2	0.9	3.40E-01
K-Q	38020	1.1	62	55.2	0.8	3.62E-01
F-T	37566	0.9	48	54.6	0.8	3.74E-01
F-W	9456	1.2	17	13.7	0.8	3.78E-01
F-K	36660	0.9	47	53.3	0.7	3.92E-01
M-Q	12015	1.2	21	17.5	0.7	3.96E-01
D-S	60686	1.1	96	88.2	0.7	4.03E-01
D-M	19320	0.9	24	28.1	0.6	4.43E-01
H-P	14168	1.2	24	20.6	0.6	4.51E-01
I-L	69156	0.9	93	100.5	0.6	4.57E-01

E-S	74564	1.1	116	108.3	0.5	4.60E-01
G-H	21942	1.1	36	31.9	0.5	4.65E-01
I-N	34402	0.9	45	50.0	0.5	4.82E-01
I-I	21194	0.9	27	30.8	0.5	4.95E-01
H-K	19778	1.1	32	28.7	0.4	5.42E-01
C-Y	13420	1.1	22	19.5	0.3	5.70E-01
M-T	20607	1.1	33	29.9	0.3	5.75E-01
F-N	25901	1.1	41	37.6	0.3	5.82E-01
A-W	17697	0.9	23	25.7	0.3	5.93E-01
V-W	18293	0.9	24	26.6	0.2	6.18E-01
M-P	14931	1.1	24	21.7	0.2	6.20E-01
A-R	46877	0.9	64	68.1	0.2	6.20E-01
M-M	4001	1.2	7	5.8	0.2	6.22E-01
H-T	20195	1.1	32	29.3	0.2	6.23E-01
Q-Q	11791	1.1	19	17.1	0.2	6.51E-01
F-L	51234	1.0	71	74.4	0.2	6.92E-01
K-R	42060	1.0	64	61.1	0.1	7.10E-01
C-F	12793	0.9	17	18.6	0.1	7.13E-01
C-G	24164	0.9	33	35.1	0.1	7.23E-01
I-R	34720	1.0	48	50.4	0.1	7.32E-01
G-G	40228	1.0	61	58.4	0.1	7.37E-01
T-T	33977	1.0	47	49.4	0.1	7.37E-01
G-T	72141	1.0	108	104.8	0.1	7.54E-01

S-S	41914	1.0	63	60.9	0.1	7.86E-01
C-W	5667	1.1	9	8.2	0.1	7.89E-01
R-V	48201	1.0	68	70.0	0.1	8.10E-01
L-Q	52287	1.0	74	76.0	0.1	8.23E-01
F-I	30741	1.0	46	44.7	0.0	8.40E-01
C-S	25630	1.0	38	37.2	0.0	9.00E-01
C-H	6645	1.0	10	9.7	0.0	9.11E-01
D-D	23855	1.0	34	34.7	0.0	9.12E-01
C-I	16712	1.0	24	24.3	0.0	9.55E-01