Supplementary Information for

Amino acid interacting network in the receptor-binding domain of SARS-CoV-2 spike protein

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This Supplementary information consists:

Figure S1 Distribution of 10 matrices (MT) in RBD with their AA sequence numbers.

Table S1: AABP matrix SD1with BL cutoff 2.500 Å and BO cutoff 0.0100 e. Pseudo-diagonal cell are highlighted with yellow.

Table S2: 10 matrices of RBD showing AABP with BL cutoff 2.500 Å and BO cutoff 0.0100 e. Pseudo-diagonal cell are highlighted with yellow.

Table S3: Contributions to the AABP from each amino acid in RBD from the inter-amino acid interaction.

Table S4: Interaction among AA with BL, BO and AABP.

Table S5: AA with chain of *off-diagonal connections* from 9 to 3 AA.

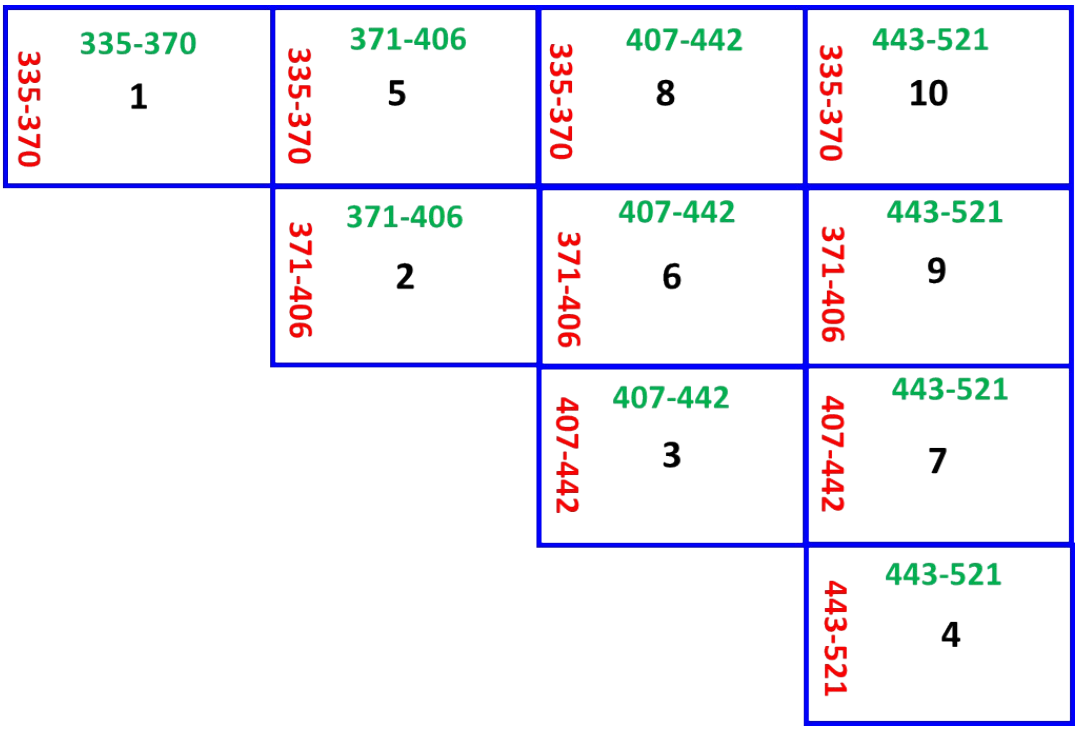

Figure S1 Sketch showing distribution of 10 matrices (MT) of RBD with their AA sequence number. (MT1) 335-370 × 335-370, (MT2) 371-406 × 371-406, (MT3) 407-442 × 407-442, (MT4) 443-521 × 443-521, (MT5) 335-370 × 371-406, (MT6) 371-406 × 407-442, (MT7) 407-442 × 443-521, (MT8) 335-370 × 407-442, (MT9) 371-406 × 443-521, (MT10) 335-370 × 443-521.

Table S1 SD1 AABP matrix with BL cutoff 2.500 Å and BO cutoff 0.0100 e. Pseudo-diagonal cell are highlighted with yellow.

		Ser	Phe	Thr	Val	Glu	Lys	Gly	Ile	Tyr	Gln	Thr	Ser	Asn	Phe	Arg	Val	Gln	Pro	Thr	Glu	Ser	Ile	Val	Arg
		305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328
Ser	305		0.399	0.079																					
Phe	306			0.432																					
Thr	307				0.496																				
Val	308					0.447																			
Glu	309						0.471			0.078															
Lys	310							0.427																	
Gly	311								0.437																
Ile	312									0.434															
Tyr	313										0.422														
Gln	314											0.403													
Thr	315												0.472												
Ser	316													0.485											
Asn	317														0.466										
Phe	318															0.444									
Arg	319																0.431								
Val	320																	0.422							
Gln	321																		0.520						
Pro	322																			0.415					
Thr	323																				0.544				
Glu	324																					0.421			
Ser	325																						0.407		
Ile	326																							0.415	
Val	327																								0.587
Arg	328																								

Table S2: 10 matrices of RBD showing AABP with BL cutoff 2.500 Å and BO cutoff 0.0100 e. Pseudo-diagonal cell are highlighted with yellow.

Matrix-1 RBD

		Leu	Cys	Pro	Phe	Gly	Glu	Val	Phe	Asn	Ala	Thr	Arg	Phe	Ala	Ser	Val	Tyr	Ala	Trp	Asn	Arg	Lys	Arg	ILE	Ser	Asn	Cys	Val	Ala	Asp	Tyr	Ser	Val	Leu	Tyr	Asn
		335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370
Leu	335		0.417																										0.104								
Cys	336			0.507	0.048																							0.173	0.033								
Pro	337				0.451		0.039																														
Phe	338					0.456		0.025																													
Gly	339						0.434			0.012																											
Glu	340							0.485															0.106														
Val	341								0.417																												
Phe	342									0.407																											
Asn	343										0.422																										
Ala	344											0.423																									
Thr	345												0.440																								
Arg	346													0.421																							
Phe	347														0.409																						
Ala	348															0.425																					
Ser	349																0.425		0.013																		
Val	350																	0.438																			
Tyr	351																		0.419																		
Ala	352																			0.421																	
Trp	353																				0.403																
Asn	354																					0.457															
Arg	355																						0.418														
Lys	356																							0.442													
Arg	357																								0.420												
ILE	358																									0.461											
Ser	359																										0.428										
Asn	360																											0.425									
Cys	361																												0.447								
Val	362																													0.449							
Ala	363																														0.553	0.047					
Asp	364																															0.445		0.025			
Tyr	365																																0.441		0.014		
Ser	366																																	0.475			0.029
Val	367																																		0.447		
Leu	368																																			0.438	
Tyr	369																																				0.405
Asn	370																																				

Matrix-2 RBD

		Ser	Ala	Ser	Phe	Ser	Thr	Phe	Lys	Cys	Tyr	Gly	Val	Ser	Pro	Thr	Lys	Leu	Asn	Asp	Leu	Cys	Phe	Thr	Asn	Val	Tyr	Ala	Asp	Ser	Phe	Val	ILE	Arg	Gly	Asp	Glu
		371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406
Ser	371		0.431	0.037																																	
Ala	372			0.397																																	
Ser	373				0.417																																
Phe	374					0.413																															
Ser	375						0.401																														
Thr	376							0.449																													
Phe	377								0.428																												
Lys	378									0.464	0.045																										
Cys	379										0.428																										
Tyr	380											0.431	0.025																								
Gly	381												0.410																								
Val	382													0.411																							
Ser	383														0.510		0.019																				
Pro	384															0.419																					
Thr	385																0.436																				
Lys	386																	0.446		0.270																	
Leu	387																		0.419																		
Asn	388																			0.424																	
Asp	389																				0.417																
Leu	390																					0.406															
Cys	391																						0.411														
Phe	392																							0.417													
Thr	393																								0.417												
Asn	394																									0.456											
Val	395																										0.457										
Tyr	396																											0.454									
Ala	397																												0.463								
Asp	398																													0.471							
Ser	399																														0.450						
Phe	400																															0.454					
Val	401																																0.422				
ILE	402																																	0.456			
Arg	403																																		0.458		0.029
Gly	404																																			0.480	
Asp	405																																				0.439
Glu	406																																				

Matrix-3 RBD

		Val	Arg	Gln	Ile	Ala	Pro	Gly	Gln	Thr	Gly	Lys	Ile	Ala	Asp	Tyr	Asn	Tyr	Lys	Leu	Pro	Asp	Asp	Phe	Thr	Gly	Cys	Val	Ile	Ala	Trp	Asn	Ser	Asn	Asn	Leu	Asp
		407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442
Val	407		0.528																																		
Arg	408			0.418																																	
Gln	409				0.435					0.038	0.015																										
Ile	410					0.485																															
Ala	411						0.499																														
Pro	412							0.399																													
Gly	413								0.420																												
Gln	414									0.408																											
Thr	415										0.447																										
Gly	416											0.439			0.010																						
Lys	417												0.446			0.016	0.012																				
Ile	418													0.449				0.026																			
Ala	419														0.430																						
Asp	420															0.405																					
Tyr	421																0.417																				
Asn	422																	0.441																			
Tyr	423																		0.422																		
Lys	424																			0.410																	
Leu	425																				0.466																
Pro	426																					0.440	0.027														
Asp	427																						0.413														
Asp	428																							0.408													
Phe	429																								0.522												
Thr	430																									0.453											
Gly	431																										0.457										
Cys	432																											0.454									
Val	433																												0.443								
Ile	434																													0.469							
Ala	435																														0.483						
Trp	436																															0.464	0.012				
Asn	437																																0.404	0.033			
Ser	438																																	0.467		0.018	0.015
Asn	439																																		0.472		
Asn	440																																			0.422	
Leu	441																																				0.403
Asp	442																																				

Matrix-4 RBD

		Ser	Tyr	Asn	Tyr	Leu	Tyr	Arg	Pro	Leu	Gln	Ser	Tyr	Gly	Phe	Gln	Pro	Thr	Val	Gly	Tyr	Gln	Pro	Tyr	Arg	Val	Val	Val	Leu	Ser	Phe	Glu	Leu	Leu	His	Ala	Pro
		443	449	450	451	452	453	454	491	492	493	494	495	496	497	498	499	500	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521
Ser	443																																				
Tyr	449			0.506								0.071																									
Asn	450				0.418																																
Tyr	451					0.418																															
Leu	452						0.439																														
Tyr	453							0.462			0.057																										
Arg	454																																				
Pro	491									0.469																											
Leu	492										0.416																										
Gln	493											0.447																									
Ser	494												0.417																								
Tyr	495													0.439	0.023																						
Gly	496														0.443	0.029																					
Phe	497															0.424																					
Gln	498																0.456																				
Pro	499																	0.437																			
Thr	500																				0.407																
Val	503																			0.939				0.109													
Gly	504																				0.503																
Tyr	505																					0.495															
Gln	506																						0.510														
Pro	507																							0.451													
Tyr	508																								0.438												
Arg	509																									0.451											
Val	510																										0.446										
Val	511																											0.453									
Val	512																												0.462								
Leu	513																													0.451							
Ser	514																														0.461						
Phe	515																															0.421					
Glu	516																																0.433				
Leu	517																																	0.397			
Leu	518																																		0.407		
His	519																																			0.428	
Ala	520																																				0.520
Pro	521																																				

Matrix-5 RBD

		Ser	Ala	Ser	Phe	Ser	Thr	Phe	Lys	Cys	Tyr	Gly	Val	Ser	Pro	Thr	Lys	Leu	Asn	Asp	Leu	Cys	Phe	Thr	Asn	Val	Tyr	Ala	Asp	Ser	Phe	Val	Ile	Arg	Gly	Asp	Glu
		371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406
Leu	335																																				
Cys	336																																				
Pro	337																																				
Phe	338																																				
Gly	339																																				
Glu	340																																				
Val	341																																				
Phe	342																																				
Asn	343																																				
Ala	344																																				
Thr	345																																				
Arg	346																																				
Phe	347																																				
Ala	348																																				
Ser	349																																				
Val	350																																				
Tyr	351																																				
Ala	352																																				
Trp	353																																				
Asn	354																													0.028							
Arg	355																																				
Lys	356																											0.054									
Arg	357																																				
Ile	358																									0.056											
Ser	359																								0.055												
Asn	360																																				
Cys	361																																				
Val	362																																				
Ala	363																																				
Asp	364																																				
Tyr	365																																				
Ser	366																																				
Val	367	0.053																																			
Leu	368																																				
Tyr	369																																				
Asn	370	0.417																																			

Matrix-6 RBD

		Val	Arg	Gln	ILE	Ala	Pro	Gly	Gln	Thr	Gly	Lys	ILE	Ala	Asp	Tyr	Asn	Tyr	Lys	Leu	Pro	Asp	Asp	Phe	Thr	Gly	Cys	Val	ILE	Ala	Trp	Asn	Ser	Asn	Asn	Leu	Asp
		407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442
Ser	371																																				
Ala	372																																				
Ser	373																																				
Phe	374																																				
Ser	375																													0.023							
Thr	376		0.030																											0.050							
Phe	377																																				
Lys	378				0.122																							0.043									
Cys	379																										0.160										
Tyr	380																									0.024											
Gly	381																																				
Val	382																																				
Ser	383																																				
Pro	384																																				
Thr	385																																				
Lys	386																																				
Leu	387																																				
Asn	388																																				
Asp	389																																				
Leu	390																																				
Cys	391																																				
Phe	392																																				
Thr	393																																				
Asn	394																																				
Val	395																																				
Tyr	396																																				
Ala	397																																				
Asp	398																																				
Ser	399																																				
Phe	400																																				
Val	401																																				
ILE	402																																				
Arg	403																																				
Gly	404	0.045																																			
Asp	405		0.025																																		
Glu	406	0.471		0.030																																	

Matrix-7 RBD

		Ser	Tyr	Asn	Tyr	Leu	Tyr	Arg	Pro	Leu	Gln	Ser	Tyr	Gly	Phe	Gln	Pro	Thr	Val	Gly	Tyr	Gln	Pro	Tyr	Arg	Val	Val	Val	Leu	Ser	Phe	Glu	Leu	Leu	His	Ala	Pro
		443	449	450	451	452	453	454	491	492	493	494	495	496	497	498	499	500	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521
Val	407																																				
Arg	408																																				
Gln	409																																				
Ile	410																																				
Ala	411																																				
Pro	412																																				
Gly	413																																				
Gln	414																																				
Thr	415																																				
Gly	416																																				
Lys	417																																				
Ile	418																																				
Ala	419																																				
Asp	420																																				
Tyr	421																																				
Asn	422							0.039																													
Tyr	423																																				
Lys	424																																				
Leu	425																																				
Pro	426																																				
Asp	427																																				
Asp	428																																				
Phe	429																																				
Thr	430																																				
Gly	431																												0.022								
Cys	432																												0.028								
Val	433																																				
Ile	434																										0.066										
Ala	435																																				
Trp	436																								0.045												
Asn	437																					0.049															
Ser	438																						0.039														
Asn	439	0.065															0.031																				
Asn	440																																				
Leu	441																																				
Asp	442	0.408			0.058																				0.139												

Matrix-8 RBD

		Val	Arg	Gln	Ile	Ala	Pro	Gly	Gln	Thr	Gly	Lys	Ile	Ala	Asp	Tyr	Asn	Tyr	Lys	Leu	Pro	Asp	Asp	Phe	Thr	Gly	Cys	Val	Ile	Ala	Trp	Asn	Ser	Asn	Asn	Leu	Asp
		407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442
Leu	335																																				
Cys	336																																				
Pro	337																																				
Phe	338																																				
Gly	339																																				
Glu	340																																				
Val	341																																				
Phe	342																																				
Asn	343																																				
Ala	344																																				
Thr	345																																				
Arg	346																																				
Phe	347																																				
Ala	348																																				
Ser	349																																				
Val	350																																				
Tyr	351																																				
Ala	352																																				
Trp	353																0.025																				
Asn	354																																				
Arg	355																	0.019																			
Lys	356																																				
Arg	357																																				
Ile	358																																				
Ser	359																																				
Asn	360																																				
Cys	361																																				
Val	362																																				
Ala	363																																				
Asp	364																																				
Tyr	365																																				
Ser	366																																				
Val	367																																				
Leu	368																																				
Tyr	369																																				
Asn	370																																				

Matrix-9 RBD

		Ser	Tyr	Asn	Tyr	Leu	Tyr	Arg	Pro	Leu	Gln	Ser	Tyr	Gly	Phe	Gln	Pro	Thr	Val	Gly	Tyr	Gln	Pro	Tyr	Arg	Val	Val	Val	Leu	Ser	Phe	Glu	Leu	Leu	His	Ala	Pro
		443	449	450	451	452	453	454	491	492	493	494	495	496	497	498	499	500	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521
Ser	371																																				
Ala	372																																				
Ser	373																																				
Phe	374																																				
Ser	375																																				
Thr	376																																				
Phe	377																																				
Lys	378																																				
Cys	379																																				
Tyr	380																																				
Gly	381																																				
Val	382																																				
Ser	383																																				
Pro	384																																				
Thr	385																																				
Lys	386																																				
Leu	387																																				
Asn	388																																				
Asp	389																																				
Leu	390																																				
Cys	391																																				
Phe	392																																				
Thr	393																															0.013				0.043	
Asn	394																															0.024					
Val	395																																				
Tyr	396																													0.041							
Ala	397																																				
Asp	398																											0.072									
Ser	399																																				
Phe	400																									0.038											
Val	401																																				
Ile	402																							0.044													
Arg	403																																				
Gly	404																					0.028															
Asp	405																			0.070																	
Glu	406																																				

Matrix-10 RBD

		Ser	Tyr	Asn	Tyr	Leu	Tyr	Arg	Pro	Leu	Gln	Ser	Tyr	Gly	Phe	Gln	Pro	Thr	Val	Gly	Tyr	Gln	Pro	Tyr	Arg	Val	Val	Val	Leu	Ser	Phe	Glu	Leu	Leu	His	Ala	Pro
		443	449	450	451	452	453	454	491	492	493	494	495	496	497	498	499	500	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521
Leu	335																																				
Cys	336																																				
Pro	337																																				
Phe	338																																				
Gly	339																																				
Glu	340																																				
Val	341																																				
Phe	342																																				
Asn	343																																				
Ala	344																								0.030												
Thr	345																								0.033												
Arg	346																																				
Phe	347																																				
Ala	348																																				
Ser	349																																				
Val	350																																				
Tyr	351																																				
Ala	352																																				
Trp	353																																				
Asn	354																																				
Arg	355																																				
Lys	356																																				
Arg	357																																				
Ile	358																																				
Ser	359																																				
Asn	360																																				
Cys	361																																				
Val	362																																				
Ala	363																																				
Asp	364																																				
Tyr	365																																				
Ser	366																																				
Val	367																																				
Leu	368																																				
Tyr	369																																				
Asn	370																																				

Table S3: Contributions to the AABP from each amino acids in RBD from the inter-amino acid interaction.

AA SeqNo.	NN	Off-Diag.	Sum	AA SeqNo.	NN	Off-Diag.	Sum	AA SeqNo.	NN	Off-Diag.	Sum	AA SeqNo.	NN	Off-Diag.	Sum
Leu335	**0.417**	**0.104**	**0.520**	Ser371	0.848	0.090	0.938	Val407	0.998	0.045	1.043	**Ser443**	**0.408**	**0.065**	**0.474**
Cys336	0.923	0.254	1.177	Ala372	0.828	-	0.828	Arg408	0.946	0.056	1.002	**Tyr449**	**0.506**	**0.071**	**0.576**
Pro337	0.958	0.039	0.997	Ser373	0.815	0.037	0.851	Gln409	0.854	0.082	0.936	Asn450	0.923	-	0.923
Phe338	0.907	0.073	0.981	Phe374	0.830	-	0.830	Ile410	0.920	0.122	1.043	Tyr451	0.836	0.058	0.894
Gly339	0.890	0.012	0.902	Ser375	0.814	0.023	0.837	Ala411	0.984	-	0.984	Leu452	0.857	-	0.857
Glu340	0.918	0.145	1.063	Thr376	0.850	0.081	0.930	Pro412	0.897	-	0.897	Tyr453	0.902	0.057	0.958
Val341	0.901	0.025	0.926	Phe377	0.876	-	0.876	Gly413	0.818	-	0.818	**Arg454**	**0.462**	**0.039**	**0.502**
Phe342	0.824	-	0.824	Lys378	0.892	0.210	1.102	Gln414	0.828	-	0.828	**Pro491**	**0.469**	**-**	**0.469**
Asn343	0.829	0.012	0.840	Cys379	0.891	0.160	1.051	Thr415	0.855	0.038	0.893	Leu492	0.886	-	0.886
Ala344	0.845	0.030	0.874	Tyr380	0.859	0.094	0.952	Gly416	0.886	0.025	0.912	Gln493	0.864	0.057	0.921
Thr345	0.863	0.033	0.896	Gly381	0.841	-	0.841	Lys417	0.885	0.029	0.914	Ser494	0.864	0.071	0.935
Arg346	0.860	-	0.860	Val382	0.820	0.025	0.845	Ile418	0.895	0.026	0.921	Tyr495	0.856	0.023	0.879
Phe347	0.830	-	0.830	Ser383	0.921	0.019	0.939	Ala419	0.879	-	0.879	Gly496	0.882	0.029	0.911
Ala348	0.834	-	0.834	Pro384	0.929	-	0.929	Asp420	0.835	0.010	0.845	Phe497	0.866	0.023	0.889
Ser349	0.850	0.013	0.863	Thr385	0.855	-	0.855	Tyr421	0.822	0.016	0.838	Gln498	0.880	0.029	0.908
Val350	0.864	-	0.864	Lys386	0.882	0.289	1.171	Asn422	0.859	0.077	0.935	Pro499	0.893	0.031	0.924
Tyr351	0.857	-	0.857	Leu387	0.865	-	0.865	Tyr423	0.863	0.045	0.908	**Thr500**	**0.437**	**0.407**	**0.845**
Ala352	0.839	0.013	0.852	Asn388	0.842	-	0.842	Lys424	0.832	-	0.832	**Val503**	**0.939**	**0.109**	**1.048**
Trp353	0.823	0.025	0.848	Asp389	0.841	0.270	1.111	Leu425	0.876	-	0.876	Gly504	1.442	0.070	1.513
Asn354	0.860	0.028	0.887	Leu390	0.823	-	0.823	Pro426	0.906	0.027	0.933	Tyr505	0.998	0.407	1.406
Arg355	0.875	0.019	0.893	Cys391	0.817	-	0.817	Asp427	0.853	-	0.853	Gln506	1.005	0.077	1.083
Lys356	0.860	0.160	1.020	Phe392	0.828	-	0.828	Asp428	0.821	0.027	0.848	Pro507	0.961	0.039	0.999
Arg357	0.862	-	0.862	Thr393	0.834	0.056	0.889	Phe429	0.930	-	0.930	Tyr508	0.889	0.152	1.041
Ile358	0.881	0.056	0.937	Asn394	0.873	0.079	0.952	Thr430	0.975	-	0.975	Arg509	0.890	0.246	1.136
Ser359	0.889	0.055	0.944	Val395	0.913	0.056	0.969	Gly431	0.910	0.046	0.955	Val510	0.897	0.038	0.935
Asn360	0.853	-	0.853	Tyr396	0.911	0.041	0.951	Cys432	0.912	0.188	1.100	Val511	0.899	0.066	0.964
Cys361	0.872	0.173	1.045	Ala397	0.917	0.054	0.971	Val433	0.897	0.043	0.940	Val512	0.914	0.072	0.986
Val362	0.896	0.136	1.032	Asp398	0.933	0.072	1.005	Ile434	0.911	0.066	0.977	Leu513	0.913	0.050	0.963
Ala363	1.002	0.047	1.050	Ser399	0.921	0.028	0.949	Ala435	0.952	0.073	1.025	Ser514	0.913	0.041	0.953
Asp364	0.998	0.025	1.023	Phe400	0.905	0.038	0.943	Trp436	0.948	0.057	1.005	Phe515	0.882	-	0.882
Tyr365	0.886	0.061	0.947	Val401	0.876	-	0.876	Asn437	0.868	0.082	0.951	Glu516	0.854	0.037	0.891
Ser366	0.916	0.029	0.945	Ile402	0.878	0.044	0.921	Ser438	0.871	0.084	0.954	Leu517	0.830	-	0.830
Val367	0.922	0.079	1.001	Arg403	0.914	0.029	0.943	Asn439	0.939	0.130	1.069	Leu518	0.804	-	0.804
Leu368	0.885	0.014	0.899	Gly404	0.938	0.073	1.011	Asn440	0.894	-	0.894	His519	0.835	-	0.835
Tyr369	0.844	-	0.844	Asp405	0.918	0.096	1.014	Leu441	0.825	0.018	0.843	Ala520	0.948	0.043	0.991
Asn370	0.822	0.029	0.851	Glu406	0.909	0.059	0.968	Asp442	0.812	0.212	1.024	**Pro521**	**0.520**	**-**	**0.520**

Table S4: Interaction among AA with BL, BO and AABP.

Bonds	BLs	BOs	AA 1	AA 2	AABP	Bonds	BLs	BOs	AA 1	AA 2	AABP
N-C	1.361	0.4166	Cys336	Leu335	0.4166	O···H	2.016	0.0203	Ile358	Val395	0.0560
N···H	1.751	0.1037	Leu335	Val362	0.1037	O···H	1.848	0.0357	Val395	Ile358	
N-C	1.363	0.5068	Pro337	Cys336	0.5068	N-C	1.358	0.4275	Asn360	Ser359	0.4275
O···H	1.780	0.0484	Cys336	Phe338	0.0484	O···H	1.800	0.0550	Asn394	Ser359	0.0550
S-S	2.025	0.1725	Cys336	Cys361	0.1725	N-C	1.352	0.4254	Cys361	Asn360	0.4254
O···H	1.864	0.0327	Val362	Cys336	0.0327	N-C	1.347	0.4467	Val362	Cys361	0.4467
N-C	1.356	0.4511	Phe338	Pro337	0.4511	N-C	1.357	0.4489	Ala363	Val362	0.4489
O···H	1.863	0.0387	Pro337	Glu340	0.0387	N-C	1.324	0.5533	Asp364	Ala363	0.5533
N-C	1.347	0.4563	Gly339	Phe338	0.4563	O···H	1.791	0.0474	Ala363	Tyr365	0.0474
O···H	1.971	0.0250	Phe338	Val341	0.0250	N-C	1.365	0.4449	Tyr365	Asp364	0.4449
N-C	1.360	0.4339	Glu340	Gly339	0.4339	O···H	2.017	0.0252	Asp364	Val367	0.0252
O···H	2.230	0.0116	Gly339	Asn343	0.0116	N-C	1.351	0.4410	Ser366	Tyr365	0.4410
N-C	1.337	0.4845	Val341	Glu340	0.4845	O···H	2.219	0.0137	Tyr365	Leu368	0.0137
O···H	1.594	0.1062	Glu340	Lys356	0.1062	N-C	1.346	0.4753	Val367	Ser366	0.4753
N-C	1.359	0.4168	Phe342	Val341	0.4168	O···H	1.871	0.0289	Ser366	Asn370	0.0289
N-C	1.363	0.4071	Asn343	Phe342	0.4071	N-C	1.356	0.4469	Leu368	Val367	0.4469
N-C	1.358	0.4215	Ala344	Asn343	0.4215	O···H	1.787	0.0533	Val367	Ser371	0.0533
N-C	1.364	0.4231	Thr345	Ala344	0.4231	N-C	1.359	0.4383	Tyr369	Leu368	0.4383
O···H	1.975	0.0297	Ala344	Arg509	0.0297	N-C	1.368	0.4052	Asn370	Tyr369	0.4052
N-C	1.358	0.4397	Arg346	Thr345	0.4397	N-C	1.359	0.4171	Ser371	Asn370	0.4171
O···H	1.921	0.0328	Thr345	Arg509	0.0328	N-C	1.361	0.4308	Ala372	Ser371	0.4308
N-C	1.354	0.4205	Phe347	Arg346	0.4205	O···H	1.906	0.0237	Ser371	Ser373	0.0366
N-C	1.366	0.4093	Ala348	Phe347	0.4093	O···H	2.148	0.0129	Ser371	Ser373	
N-C	1.355	0.4247	Ser349	Ala348	0.4247	N-C	1.368	0.3972	Ser373	Ala372	0.3972
N-C	1.357	0.4254	Val350	Ser349	0.4254	N-C	1.363	0.4174	Phe374	Ser373	0.4174
O···H	2.191	0.0126	Ser349	Ala352	0.0126	N-C	1.372	0.4126	Ser375	Phe374	0.4126
N-C	1.355	0.4381	Tyr351	Val350	0.4381	N-C	1.380	0.4013	Thr376	Ser375	0.4013
N-C	1.360	0.4186	Ala352	Tyr351	0.4186	O···H	1.999	0.0228	Ala435	Ser375	0.0228
N-C	1.359	0.4208	Trp353	Ala352	0.4208	N-C	1.350	0.4485	Phe377	Thr376	0.4485
N-C	1.374	0.4025	Asn354	Trp353	0.4025	O···H	1.841	0.0303	Thr376	Arg408	0.0303
O···H	1.950	0.0248	Asn422	Trp353	0.0248	O···H	1.959	0.0276	Thr376	Ala435	0.0503
N-C	1.349	0.4572	Arg355	Asn354	0.4572	O···H	1.967	0.0227	Ala435	Thr376	
O···H	1.962	0.0276	Asn354	Ser399	0.0276	N-C	1.355	0.4278	Lys378	Phe377	0.4278
N-C	1.359	0.4176	Lys356	Arg355	0.4176	N-C	1.351	0.4638	Cys379	Lys378	0.4638
O···H	1.957	0.0185	Tyr423	Arg355	0.0185	O···H	1.847	0.0449	Tyr380	Lys378	0.0449
N-C	1.355	0.4420	Arg357	Lys356	0.4420	O···H	1.567	0.1221	Ile410	Lys378	0.1221
O···H	1.991	0.0238	Lys356	Ala397	0.0538	O···H	1.878	0.0294	Lys378	Val433	0.0430
O···H	1.901	0.0300	Ala397	Lys356		O···H	2.148	0.0136	Val433	Lys378	
N-C	1.346	0.4201	Ile358	Arg357	0.4201	N-C	1.354	0.4276	Tyr380	Cys379	0.4276
N-C	1.345	0.4613	Ser359	Ile358	0.4613	S-S	2.037	0.1599	Cys379	Cys432	0.1599

Bonds	BLs	BOs	AA 1	AA 2	AABP	Bonds	BLs	BOs	AA 1	AA 2	AABP
N-C	1.358	0.4312	Gly381	Tyr380	0.4312	O···H	1.773	0.0449	Gly404	Val407	0.0449
O···H	2.003	0.0248	Tyr380	Val382	0.0248	O···H	1.936	0.0283	Gln506	Gly404	0.0283
O···H	1.951	0.0239	Gly431	Tyr380	0.0239	N-C	1.355	0.4386	Glu406	Asp405	0.4386
N-C	1.359	0.4097	Val382	Gly381	0.4097	O···H	2.046	0.0252	Asp405	Arg408	0.0252
N-C	1.359	0.4107	Ser383	Val382	0.4107	O···H	1.664	0.0704	Gly504	Asp405	0.0704
N-C	1.354	0.5098	Pro384	Ser383	0.5098	N-C	1.345	0.4705	Val407	Glu406	0.4705
O···H	2.100	0.0187	Ser383	Lys386	0.0187	O···H	1.896	0.0297	Glu406	Gln409	0.0297
N-C	1.358	0.4188	Thr385	Pro384	0.4188	O···H	1.870	0.0390	Val407	Arg408	0.5279
N-C	1.357	0.4358	Lys386	Thr385	0.4358	O···H	2.060	0.0217	Val407	Arg408	
N-C	1.359	0.4459	Leu387	Lys386	0.4459	N-C	1.348	0.4672	Arg408	Val407	
O···H	2.141	0.0149	Lys386	Asp389	0.2704	N-C	1.365	0.4183	Gln409	Arg408	0.4183
O-H	1.030	0.2555	Asp389	Lys386		N-C	1.363	0.4354	Ile410	Gln409	0.4354
N-C	1.359	0.4188	Asn388	Leu387	0.4188	O···H	1.875	0.0375	Thr415	Gln409	0.0375
N-C	1.363	0.4236	Asp389	Asn388	0.4236	O···H	2.196	0.0151	Gln409	Gly416	0.0151
N-C	1.361	0.4172	Leu390	Asp389	0.4172	N-C	1.337	0.4850	Ala411	Ile410	0.4850
N-C	1.370	0.4060	Cys391	Leu390	0.4060	N-C	1.347	0.4985	Pro412	Ala411	0.4985
N-C	1.359	0.4110	Phe392	Cys391	0.4110	N-C	1.362	0.3986	Gly413	Pro412	0.3986
N-C	1.359	0.4169	Thr393	Phe392	0.4169	N-C	1.357	0.4198	Gln414	Gly413	0.4198
N-C	1.370	0.4167	Asn394	Thr393	0.4167	N-C	1.365	0.4077	Thr415	Gln414	0.4077
O···H	2.148	0.0133	Glu516	Thr393	0.0133	N-C	1.352	0.4474	Gly416	Thr415	0.4474
O···H	1.835	0.0425	Ala520	Thr393	0.0425	N-C	1.358	0.4390	Lys417	Gly416	0.4390
N-C	1.345	0.4562	Val395	Asn394	0.4562	O···H	2.257	0.0102	Gly416	Asp420	0.0102
O···H	1.947	0.0238	Asn394	Glu516	0.0238	N-C	1.353	0.4462	Ile418	Lys417	0.4462
N-C	1.355	0.4565	Tyr396	Val395	0.4565	O···H	2.095	0.0161	Lys417	Tyr421	0.0161
N-C	1.348	0.4541	Ala397	Tyr396	0.4541	O···H	2.251	0.0124	Lys417	Asn422	0.0124
O···H	1.926	0.0279	Tyr396	Ser514	0.0406	N-C	1.352	0.4489	Ala419	Ile418	0.4489
O···H	2.139	0.0127	Ser514	Tyr396		O···H	1.909	0.0263	Ile418	Tyr423	0.0263
N-C	1.344	0.4627	Asp398	Ala397	0.4627	N-C	1.360	0.4299	Asp420	Ala419	0.4299
N-C	1.345	0.4706	Ser399	Asp398	0.4706	N-C	1.370	0.4046	Tyr421	Asp420	0.4046
O···H	1.824	0.0389	Asp398	Val512	0.0720	N-C	1.369	0.4174	Asn422	Tyr421	0.4174
O···H	1.902	0.0331	Val512	Asp398		N-C	1.361	0.4412	Tyr423	Asn422	0.4412
N-C	1.347	0.4504	Phe400	Ser399	0.4504	O···H	1.943	0.0393	Asn422	Arg454	0.0393
N-C	1.350	0.4544	Val401	Phe400	0.4544	N-C	1.356	0.4217	Lys424	Tyr423	0.4217
O···H	1.940	0.0241	Phe400	Val510	0.0381	N-C	1.363	0.4103	Leu425	Lys424	0.4103
O···H	2.192	0.0140	Val510	Phe400		N-C	1.361	0.4656	Pro426	Leu425	0.4656
N-C	1.358	0.4220	Ile402	Val401	0.4220	N-C	1.357	0.4404	Asp427	Pro426	0.4404
N-C	1.354	0.4556	Arg403	Ile402	0.4556	O···H	1.957	0.0273	Pro426	Asp428	0.0273
O···H	1.884	0.0295	Ile402	Tyr508	0.0435	N-C	1.360	0.4127	Asp428	Asp427	0.4127
O···H	2.196	0.0140	Tyr508	Ile402		N-C	1.367	0.4079	Phe429	Asp428	0.4079
N-C	1.343	0.4584	Gly404	Arg403	0.4584	O···H	1.787	0.0596	Phe429	Thr430	0.5220
O···H	1.953	0.0289	Arg403	Glu406	0.0289	N-C	1.343	0.4624	Thr430	Phe429	
N-C	1.344	0.4798	Asp405	Gly404	0.4798	N-C	1.350	0.4525	Gly431	Thr430	0.4525

Bonds	BLs	BOs	AA 1	AA 2	AABP	Bonds	BLs	BOs	AA 1	AA 2	AABP
N-C	1.354	0.4572	Cys432	Gly431	0.4572	O···H	1.872	0.0303	Tyr453	Gln493	0.0568
O···H	2.054	0.0217	Leu513	Gly431	0.0217	O···H	1.940	0.0265	Gln493	Tyr453	
N-C	1.346	0.4543	Val433	Cys432	0.4543	N···H	2.144	0.0394	Pro491	Leu492	0.4692
O···H	1.918	0.0282	Cys432	Leu513	0.0282	N-C	1.345	0.4298	Leu492	Pro491	
N-C	1.343	0.4426	Ile434	Val433	0.4426	N-C	1.358	0.4163	Gln493	Leu492	0.4163
N-C	1.349	0.4688	Ala435	Ile434	0.4688	N-C	1.354	0.4474	Ser494	Gln493	0.4474
O···H	1.853	0.0347	Ile434	Val511	0.0655	N-C	1.358	0.4170	Tyr495	Ser494	0.4170
O···H	1.921	0.0308	Val511	Ile434		N-C	1.357	0.4392	Gly496	Tyr495	0.4392
N-C	1.343	0.4831	Trp436	Ala435	0.4831	O···H	2.037	0.0225	Tyr495	Phe497	0.0225
N-C	1.348	0.4644	Asn437	Trp436	0.4644	N-C	1.355	0.4428	Phe497	Gly496	0.4428
O···H	2.278	0.0119	Trp436	Ser438	0.0119	O···H	1.982	0.0286	Gly496	Gln498	0.0286
O···H	1.988	0.0238	Trp436	Arg509	0.0452	N-C	1.353	0.4236	Gln498	Phe497	0.4236
O···H	2.059	0.0214	Arg509	Trp436		N-C	1.372	0.4562	Pro499	Gln498	0.4562
N-C	1.353	0.4039	Ser438	Asn437	0.4039	N-C	1.354	0.4372	Thr500	Pro499	0.4372
O···H	1.889	0.0331	Asn437	Asn439	0.0331	C-H	1.118	0.4074	Thr500	Tyr505	0.4074
O···H	1.780	0.0491	Gln506	Asn437	0.0491	N-H	1.024	0.3395	Val503	Gly504	0.9390
N-C	1.352	0.4670	Asn439	Ser438	0.4670	N-C	1.316	0.5995	Gly504	Val503	
O···H	2.044	0.0177	Ser438	Leu441	0.0177	O···H	1.505	0.1089	Val503	Tyr508	0.1089
O···H	2.071	0.0154	Ser438	Asp442	0.0154	N···H	2.042	0.0367	Gly504	Tyr505	0.5032
O···H	1.841	0.0385	Pro507	Ser438	0.0385	N-C	1.344	0.4665	Tyr505	Gly504	
O···H	2.030	0.0235	Asn439	Asn440	0.4721	O···H	1.704	0.0688	Tyr505	Gln506	0.4952
N-C	1.342	0.4486	Asn440	Asn439		N-C	1.355	0.4264	Gln506	Tyr505	
O···H	1.768	0.0654	Asn439	Ser443	0.0654	N-C	1.355	0.5101	Pro507	Gln506	0.5101
O···H	1.967	0.0310	Pro499	Asn439	0.0310	N-C	1.351	0.4505	Tyr508	Pro507	0.4505
N-C	1.360	0.4221	Leu441	Asn440	0.4221	N-C	1.353	0.4384	Arg509	Tyr508	0.4384
N-C	1.373	0.4032	Asp442	Leu441	0.4032	N-C	1.352	0.4513	Val510	Arg509	0.4513
N-C	1.371	0.4084	Ser443	Asp442	0.4084	N-C	1.354	0.4460	Val511	Val510	0.4460
O···H	1.686	0.0580	Asp442	Tyr451	0.0580	N-C	1.353	0.4526	Val512	Val511	0.4526
O···H	1.652	0.0836	Asp442	Arg509	0.1386	N-C	1.353	0.4617	Leu513	Val512	0.4617
O···H	1.769	0.0550	Asp442	Arg509		N-C	1.355	0.4513	Ser514	Leu513	0.4513
N···H	1.954	0.0499	Tyr449	Asn450	0.5055	N-C	1.342	0.4614	Phe515	Ser514	0.4614
N-C	1.348	0.4556	Asn450	Tyr449		N-C	1.357	0.4205	Glu516	Phe515	0.4205
O···H	1.736	0.0705	Tyr449	Ser494	0.0705	N-C	1.351	0.4333	Leu517	Glu516	0.4333
N-C	1.354	0.4178	Tyr451	Asn450	0.4178	N-C	1.362	0.3970	Leu518	Leu517	0.3970
N-C	1.358	0.4180	Leu452	Tyr451	0.4180	N-C	1.365	0.4069	His519	Leu518	0.4069
N-C	1.353	0.4393	Tyr453	Leu452	0.4393	N-C	1.353	0.4284	Ala520	His519	0.4284
N-C	1.355	0.4622	Arg454	Tyr453	0.4622	N-C	1.349	0.5197	Pro521	Ala520	0.5197

Table S5: AA with chain of *off-diagonal connections* from 9 to 3 AA.

Unique *off-diagonal connections*									**Count**
Ala344	Arg509	Asp442	Leu441	Pro507	Ser438	Thr345	Trp436	Tyr451	9
Cys379	Cys432	Gly431	Ile410	Leu513	Lys378	Tyr380	Val382	Val433	9
Asn437	Asn439	Gln506	Gly404	Pro499	Ser443	Val407			7
Cys336	Cys361	Leu335	Phe338	Val341	Val362				6
Ala435	Arg408	Asp405	Gly504	Ser375	Thr376				6
Arg403	Asp420	Gln409	Glu406	Gly416	Thr415				6
Arg454	Asn422	Lys417	Trp353	Tyr421					5
Ala520	Asn394	Glu516	Ser359	Thr393					5
Ala397	Glu340	Lys356	Pro337						4
Asp364	Ser371	Ser373	Val367						4
Arg355	Ile418	Tyr423							3
Ala363	Leu368	Tyr365							3
Asp389	Lys386	Ser383							3
Ile402	Tyr508	Val503							3