Electronic Supplementary Information for

Intra- and intermolecular atomic-scale interactions in the receptor binding domain of SARS-CoV-2 spike protein: implication for ACE2 receptor binding

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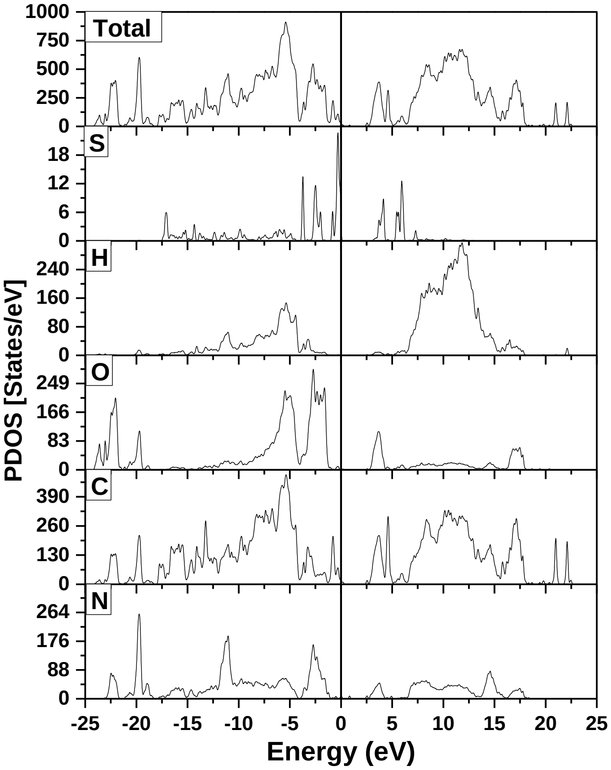

Figure S1. Total and atom-resolved partial DOS in RBD.

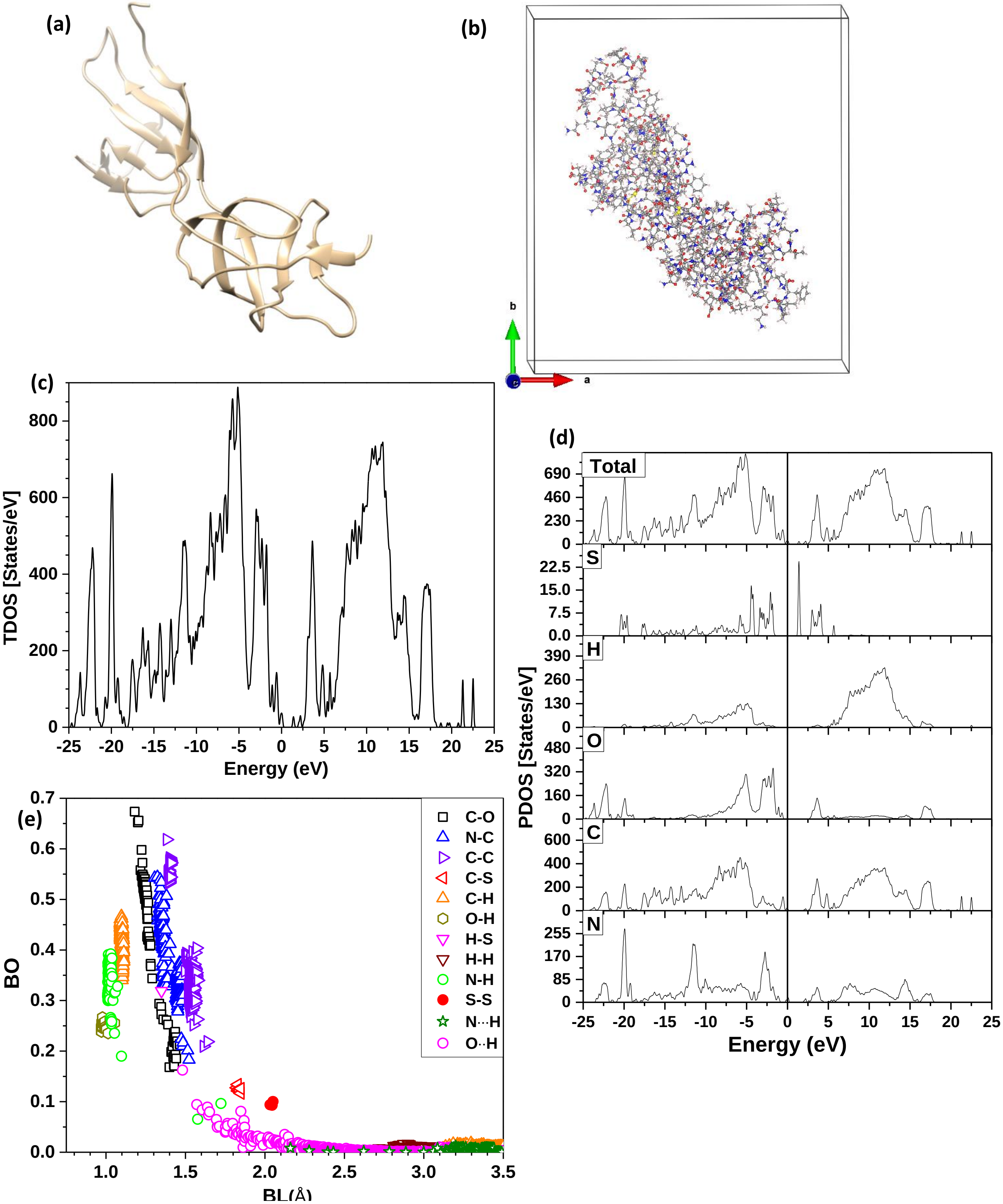

Figure S2. **(a)** Ribbon structure of SD1-SD2 , **(b)** ball-and-stick sketch of SD1-SD2 (grey: C, red: O, white: H, blue: N, and yellow: S), **(c)** TDOS of SD1-SD2, **(d)** atom-resolved PDOS of SD1-SD2, **(e)** BO vs. BL for all interatomic pairs in SD1-SD2.

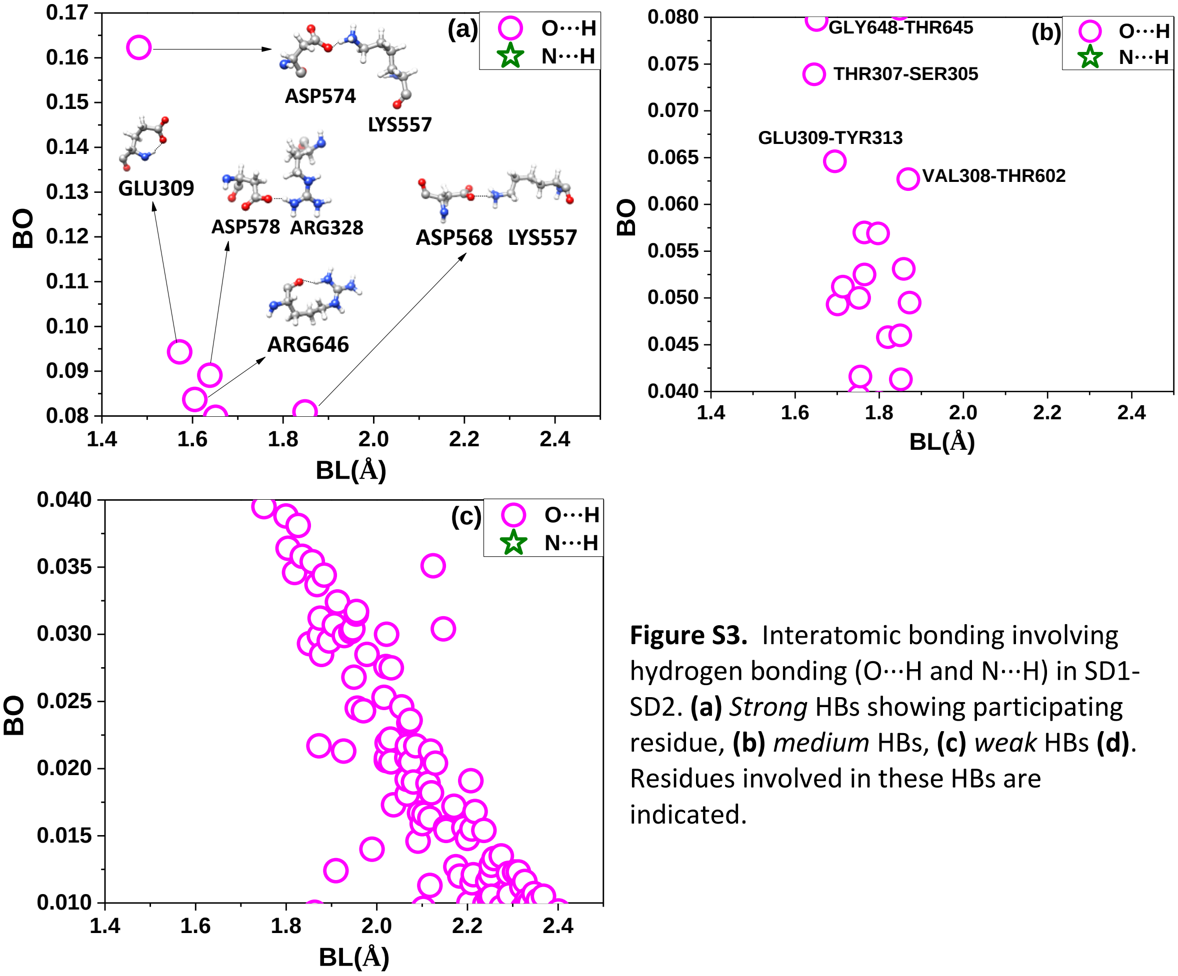

Figure S3. Interatomic bonding involving hydrogen bonding (O···H and N···H) in SD1-SD2. **(a)** *Strong* HBs showing participating residue, **(b)** *medium* HBs, **(c)** *weak* HBs **(d)**. Residues involved in these HBs are indicated.

Table S1: List of PC in sequence order of AA in the RBD. Color coded according to **Figure 2**.

AA & Seq No	PC	AA & Seq No	PC	AA & Seq No	PC	AA & Seq No	PC
LEU335	-0.789	PHE374	0.004	GLY413	0.002	GLN493	-0.028
CYS336	-0.139	SER375	-0.018	GLN414	-0.008	SER494	-0.103
PRO337	0.136	THR376	-0.039	THR415	-0.008	TYR495	-0.029
PHE338	-0.050	PHE377	0.027	GLY416	0.022	GLY496	0.064
GLY339	0.092	LYS378	0.742	LYS417	0.051	PHE497	0.010
GLU340	0.025	CYS379	0.028	ILE418	0.031	GLN498	-0.073
VAL341	0.032	TYR380	0.023	ALA419	0.052	PRO499	0.053
PHE342	0.008	GLY381	0.073	ASP420	0.027	THR500	-0.257
ASN343	-0.035	VAL382	-0.049	TYR421	-0.062	VAL503	-0.909
ALA344	0.032	SER383	-0.113	ASN422	0.015	GLY504	0.227
THR345	0.023	PRO384	0.145	TYR423	0.009	TYR505	-0.575
ARG346	0.030	THR385	-0.013	LYS424	0.012	GLN506	-0.093
PHE347	0.034	LYS386	0.465	LEU425	-0.063	PRO507	0.145
ALA348	-0.036	LEU387	-0.004	PRO426	0.051	TYR508	-0.219
SER349	0.017	ASN388	0.021	ASP427	0.054	ARG509	0.660
VAL350	-0.032	ASP389	-0.498	ASP428	-0.029	VAL510	-0.010
TYR351	0.044	LEU390	-0.005	PHE429	0.013	VAL511	-0.022
ALA352	-0.029	CYS391	-0.004	THR430	-0.085	VAL512	-0.038
TRP353	-0.021	PHE392	-0.013	GLY431	0.020	LEU513	0.011
ASN354	-0.057	THR393	-0.108	CYS432	0.068	SER514	-0.051
ARG355	1.005	ASN394	0.096	VAL433	-0.035	PHE515	0.083
LYS356	0.818	VAL395	0.010	ILE434	-0.026	GLU516	-0.042
ARG357	-1.007	TYR396	0.023	ALA435	-0.011	LEU517	0.037
ILE358	-0.096	ALA397	0.010	TRP436	0.067	LEU518	0.020
SER359	-0.046	ASP398	-0.012	ASN437	0.073	HIS519	-0.020
ASN360	0.044	SER399	-0.015	SER438	-0.118	ALA520	-0.084
CYS361	-0.039	PHE400	0.029	ASN439	0.070	PRO521	1.170
VAL362	-0.130	VAL401	0.028	ASN440	-0.008		
ALA363	-0.259	ILE402	-0.033	LEU441	-0.008		
ASP364	-0.595	ARG403	0.052	ASP442	-0.701		
TYR365	-0.056	GLY404	-0.022	SER443	0.885		
SER366	0.045	ASP405	-0.006	TYR449	-0.898		
VAL367	0.088	GLU406	-0.050	ASN450	-0.010		
LEU368	-0.009	VAL407	0.053	TYR451	-0.065		
TYR369	0.020	ARG408	0.884	LEU452	-0.023		
ASN370	-0.073	GLN409	-0.117	TYR453	-0.029		
SER371	-0.055	ILE410	0.069	ARG454	1.054		
ALA372	0.078	ALA411	0.005	PRO491	-0.973		
SER373	-0.098	PRO412	0.108	LEU492	-0.037		

Table S2: List of PC in sequence order of AA in the SD1-SD2. Color coded as **Figure 5**.

AA& Seq No	PC	AA& Seq No	PC	AA & Seq No	PC	AA & Seq No	PC
SER305	-1.094	LYS537	0.475	VAL576	0.009	VAL615	-0.046
PHE306	-0.008	CYS538	0.009	ARG577	0.808	ASN616	0.053
THR307	-0.013	VAL539	-0.010	ASP578	-0.795	CYS617	0.010
VAL308	0.091	ASN540	-0.023	PRO579	0.119	THR618	-0.093
GLU309	-0.845	PHE541	0.083	GLN580	-0.014	GLU619	-0.802
LYS310	0.552	ASN542	-0.003	THR581	0.028	VAL620	0.955
GLY311	-0.008	PHE543	-0.048	LEU582	-0.064	SER640	0.982
ILE312	-0.020	ASN544	0.080	GLU583	-1.050	ASN641	-0.003
TYR313	-0.123	GLY545	0.002	ILE584	0.019	VAL642	0.064
GLN314	0.084	LEU546	-0.063	LEU585	-0.047	PHE643	0.022
THR315	-0.079	THR547	0.068	ASP586	-0.939	GLN644	0.053
SER316	0.004	GLY548	0.001	ILE587	-0.033	THR645	-0.101
ASN317	-0.035	THR549	0.013	THR588	-0.134	ARG646	0.931
PHE318	0.015	GLY550	-0.010	PRO589	0.204	ALA647	0.053
ARG319	0.972	VAL551	-0.034	CYS590	0.034	GLY648	0.036
VAL320	-0.006	LEU552	0.023	SER591	-0.048	CYS649	0.069
GLN321	-0.094	THR553	0.060	PHE592	-0.046	LEU650	-0.035
PRO322	0.110	GLU554	-0.991	GLY593	0.018	ILE651	-0.024
THR323	-0.081	SER555	0.049	GLY594	0.069	GLY652	0.004
GLU324	-0.471	ASN556	-0.011	VAL595	-0.004	ALA653	-0.008
SER325	-0.045	LYS557	0.566	SER596	-0.001	GLU654	-0.988
ILE326	-0.054	LYS558	0.979	VAL597	-0.004	HIS655	0.008
VAL327	-0.017	PHE559	0.045	ILE598	-0.036	VAL656	-0.018
ARG328	1.732	LEU560	-0.135	THR599	-0.050	ASN657	-0.005
ALA522	1.003	PRO561	0.139	PRO600	0.137	ASN658	0.028
THR523	-0.007	PHE562	-0.007	GLY601	0.018	SER659	-0.045
VAL524	0.004	GLN563	-0.030	THR602	-0.051	TYR660	0.013
CYS525	-0.017	GLN564	0.142	ASN603	0.009	GLU661	-0.875
GLY526	-0.038	PHE565	0.000	THR604	-0.079	CYS662	-0.074
PRO527	0.056	GLY566	-0.005	SER605	-0.023	ASP663	-0.477
LYS528	-0.019	ARG567	0.459	ASN606	0.006	ILE664	-0.155
LYS529	0.088	ASP568	-0.786	GLN607	-0.011	PRO665	0.239
SER530	-0.041	ILE569	0.020	VAL608	-0.018	ILE666	-0.054
THR531	-0.082	ALA570	0.095	ALA609	-0.014	GLY667	-0.020
ASN532	0.144	ASP571	-0.516	VAL610	0.005	ALA668	0.032
LEU533	-0.003	THR572	-0.104	LEU611	-0.042	GLY669	0.014
VAL534	-0.026	THR573	-0.036	TYR612	0.031	ILE670	-0.035
LYS535	0.942	ASP574	-0.704	GLN613	0.014	CYS671	-0.025
ASN536	-0.032	ALA575	0.025	ASP614	-1.008	ALA672	0.949

Table S3: List of HBs in RBD with participating residues in the decreasing order of BO. Pink: O···H & green: N···H.

BL(Å)	BO(e)	AA & Seq No	AA & Seq No	BL(Å)	BO(e)	AA & Seq No	AA & Seq No	BL(Å)	BO(e)	AA & Seq No	AA & Seq No
1.567	0.122	ILE410	LYS378	1.902	0.033	VAL512	ASP398	1.906	0.024	SER371	SER373
1.505	0.109	VAL503	TYR508	1.921	0.033	THR345	ARG509	2.030	0.024	ASN439	ASN440
1.594	0.106	GLU340	LYS356	2.037	0.033	SER383	SER383	1.999	0.023	ALA435	SER375
1.751	0.104	LEU335	VAL362	1.864	0.033	VAL362	CYS336	1.967	0.023	ALA435	THR376
1.652	0.084	ASP442	ARG509	1.967	0.031	PRO499	ASN439	2.037	0.023	TYR495	PHE497
1.736	0.071	TYR449	SER494	1.921	0.031	VAL511	ILE434	2.054	0.022	LEU513	GLY431
1.664	0.070	GLY504	ASP405	1.963	0.031	THR430	THR430	2.060	0.022	VAL407	ARG408
1.704	0.069	TYR505	GLN506	1.841	0.030	THR376	ARG408	2.059	0.021	ARG509	TRP436
1.768	0.065	ASN439	SER443	1.872	0.030	TYR453	GLN493	2.105	0.021	SER359	SER359
1.787	0.060	PHE429	THR430	1.901	0.030	ALA397	LYS356	2.111	0.021	CYS361	CYS361
1.686	0.058	ASP442	TYR451	1.896	0.030	GLU406	GLN409	2.016	0.020	ILE358	VAL395
1.769	0.055	ASP442	ARG509	1.975	0.030	ALA344	ARG509	2.100	0.019	SER383	LYS386
1.800	0.055	ASN394	SER359	1.884	0.030	ILE402	TYR508	1.957	0.019	TYR423	ARG355
1.787	0.053	VAL367	SER371	1.878	0.029	LYS378	VAL433	2.088	0.018	ALA520	ALA520
1.954	0.050	TYR449	ASN450	1.871	0.029	SER366	ASN370	2.044	0.018	SER438	LEU441
1.780	0.049	GLN506	ASN437	1.953	0.029	ARG403	GLU406	2.095	0.016	LYS417	TYR421
1.780	0.048	CYS336	PHE338	1.982	0.029	GLY496	GLN498	2.205	0.016	GLY416	GLY416
1.791	0.047	ALA363	TYR365	1.936	0.028	GLN506	GLY404	2.071	0.015	SER438	ASP442
1.886	0.046	THR385	THR385	1.918	0.028	CYS432	LEU513	2.196	0.015	GLN409	GLY416
1.773	0.045	GLY404	VAL407	1.926	0.028	TYR396	SER514	2.141	0.015	LYS386	ASP389
1.847	0.045	TYR380	LYS378	1.959	0.028	THR376	ALA435	2.216	0.015	CYS379	CYS379
1.835	0.043	ALA520	THR393	1.962	0.028	ASN354	SER399	2.196	0.015	ALA411	ALA411
1.917	0.042	SER514	SER514	1.957	0.027	PRO426	ASP428	2.192	0.014	VAL510	PHE400
1.969	0.041	THR500	THR500	1.940	0.027	GLN493	TYR453	2.196	0.014	TYR508	ILE402
2.144	0.039	PRO491	LEU492	1.909	0.026	ILE418	TYR423	2.219	0.014	TYR365	LEU368
1.943	0.039	ASN422	ARG454	2.017	0.025	ASP364	VAL367	2.148	0.014	VAL433	LYS378
1.870	0.039	VAL407	ARG408	2.046	0.025	ASP405	ARG408	2.148	0.013	GLU516	THR393
1.824	0.039	ASP398	VAL512	1.971	0.025	PHE338	VAL341	2.148	0.013	SER371	SER373
1.863	0.039	PRO337	GLU340	1.950	0.025	ASN422	TRP353	2.139	0.013	SER514	TYR396
1.841	0.039	PRO507	SER438	2.003	0.025	TYR380	VAL382	2.191	0.013	SER349	ALA352
1.875	0.038	THR415	GLN409	1.940	0.024	PHE400	VAL510	2.243	0.013	PHE400	PHE400
2.042	0.037	GLY504	TYR505	1.951	0.024	GLY431	TYR380	2.251	0.012	LYS417	ASN422
1.848	0.036	VAL395	ILE358	1.947	0.024	ASN394	GLU516	2.204	0.012	PHE429	PHE429
1.853	0.035	ILE434	VAL511	1.988	0.024	TRP436	ARG509	2.278	0.012	TRP436	SER438
1.889	0.033	ASN437	ASN439	1.991	0.024	LYS356	ALA397	2.230	0.012	GLY339	ASN343

Table S4: List of HBs in SD1-SD2 with participating residues in the decreasing order of BO. Pink: O⋯H & green: N⋯H.

BL(Å)	BO(e)	AA & Seq No	AA & Seq No	BL(Å)	BO(e)	AA & Seq No	AA & Seq No	BL(Å)	BO(e)	AA & Seq No	AA & Seq No
1.482	0.162	ASP574	LYS557	2.147	0.030	THR553	LYS535	2.037	0.017	GLY601	THR604
1.572	0.094	GLU309	GLU309	1.943	0.030	GLN563	ARG577	2.171	0.017	ARG319	ARG319
1.638	0.089	ASP578	ARG328	2.022	0.030	VAL327	ARG328	2.217	0.017	VAL534	VAL534
1.605	0.084	ARG646	ARG646	1.874	0.030	VAL576	LEU585	2.095	0.017	ILE326	ASN542
1.849	0.081	ASP568	LYS557	1.929	0.030	PHE643	LEU650	2.104	0.017	GLY594	GLN613
1.651	0.080	GLY648	THR645	1.895	0.030	CYS649	TYR612	2.117	0.016	GLY311	THR599
1.646	0.074	THR307	SER305	1.852	0.029	THR581	ARG328	2.100	0.016	THR307	THR307
1.695	0.065	GLU309	TYR313	1.878	0.029	ALA575	GLY566	2.152	0.016	PHE541	GLY548
1.869	0.063	VAL308	THR602	1.978	0.029	LEU611	SER596	2.192	0.016	ARG567	ARG567
1.765	0.057	ILE569	THR572	2.020	0.028	PHE592	PHE592	2.210	0.016	LYS528	SER530
1.797	0.057	GLN564	ARG577	2.032	0.028	PHE565	PHE565	2.153	0.015	ARG328	GLN580
1.858	0.053	ASN532	THR531	1.950	0.027	GLY593	ASN317	2.237	0.015	ASN317	SER316
1.765	0.053	GLU619	THR618	2.016	0.025	ALA647	ASP614	2.200	0.015	LYS528	SER530
1.714	0.051	ILE664	ALA672	2.055	0.025	ASP578	LEU582	2.091	0.015	ILE569	THR572
1.752	0.050	GLU661	CYS662	1.957	0.025	ASN532	LEU533	1.989	0.014	THR531	VAL327
1.872	0.050	THR573	THR573	1.971	0.024	GLY548	PHE541	2.275	0.014	GLU661	ASP663
1.701	0.049	LEU546	PHE543	2.074	0.024	VAL327	THR531	2.259	0.013	SER316	SER316
1.850	0.046	GLU619	SER591	2.071	0.023	CYS525	CYS525	2.253	0.013	GLY550	GLY550
1.821	0.046	THR531	ARG328	2.030	0.022	GLN564	ARG577	2.175	0.013	GLU619	GLU619
1.755	0.042	ASN542	ARG328	2.023	0.022	SER591	VAL320	1.910	0.012	THR553	GLU554
1.851	0.041	ASN540	SER325	1.872	0.022	THR645	ALA647	3.200	0.012	ARG567	ARG567
1.751	0.040	THR588	VAL551	2.068	0.022	VAL597	TYR313	2.304	0.012	ASN317	ASN317
1.800	0.039	SER596	LEU611	2.086	0.022	ILE598	ALA609	2.313	0.012	THR549	THR549
1.826	0.038	ALA609	ILE598	1.927	0.021	VAL308	THR602	2.291	0.012	SER605	SER605
1.804	0.036	ASP574	ILE587	2.119	0.021	ASN616	CYS617	2.213	0.012	GLN613	VAL615
1.836	0.036	VAL610	ILE651	2.021	0.021	ASN616	VAL615	2.252	0.012	GLY593	GLY593
1.858	0.035	LEU585	VAL576	2.066	0.021	ASN603	ASN603	2.184	0.012	ASN658	ASN658
2.125	0.035	ASP568	LYS557	2.021	0.021	LEU650	PHE643	2.245	0.012	TYR612	CYS649
1.819	0.035	LEU552	ASN536	2.031	0.021	GLU583	ASP578	2.327	0.012	LEU560	GLN563
1.884	0.034	TYR313	VAL597	2.075	0.021	VAL551	THR588	2.210	0.012	THR645	GLY648
1.868	0.034	PHE543	LEU546	2.130	0.020	TYR660	TYR660	2.117	0.011	GLY601	SER605
1.913	0.032	ILE651	VAL610	2.067	0.019	GLY667	ILE670	2.320	0.011	CYS671	CYS671
1.955	0.032	CYS538	THR323	2.208	0.019	PRO600	THR604	2.347	0.011	VAL524	VAL524
1.955	0.032	ASP586	THR553	2.081	0.019	ILE670	GLY667	2.292	0.011	VAL539	GLY550
1.875	0.031	GLY550	VAL539	2.113	0.019	ILE670	ILE666	2.253	0.011	SER316	VAL595
1.907	0.031	ASP578	GLU583	2.121	0.018	VAL595	THR315	2.368	0.011	SER659	SER659
1.947	0.030	ASN641	GLY652	2.067	0.018	THR599	GLY311	3.197	0.011	ARG577	ARG577