Extracting the Electrostatic Features from COVID-19 Coronavirus-Related Experimental Structures inside Protein Data Bank: Supplementary Materials

Wei Li*

March 3, 2020

*Institute of Special Environment Medicine, Nantong University, No. 9, Seyuan Road, Nantong City, Jiangsu Province, P. R. China

List of Tables

Supporting Material

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LU7	A_LYS_5	NZ	A_GLU_288	OE1	3.977
6LU7	A_ARG_40	NH2	A_ASP_187	OD1	3.040
6LU7	A_ARG_40	NH2	A_ASP_187	OD2	3.380
6LU7	A_ARG_60	NH2	A_ASP_56	OD2	3.978
6LU7	A_ARG_76	NH2	A_ASP_92	OD1	2.923
6LU7	A_ARG_76	NH2	A_ASP_92	OD2	3.767
6LU7	A_ARG_105	NH1	A_ASP_176	OD1	3.990
6LU7	A_ARG_105	NH1	A_ASP_176	OD2	2.771
6LU7	A_ARG_131	NH1	A_ASP_289	OD1	2.939
6LU7	A_ARG_131	NH1	A_ASP_289	OD2	2.873
6LU7	A_ARG_131	NH1	A_GLU_290	OE2	3.231
6LU7	A_ARG_131	NH2	A_ASP_197	OD2	3.526
6LU7	A_ARG_131	NH2	A_ASP_289	OD1	3.835
6LU7	A_ARG_131	NH2	A_ASP_289	OD2	2.581
6LU7	A_LYS_137	NZ	A_ASP_197	OD2	3.803
6LU7	A_HIS_172	NE2	A_GLU_166	OE2	2.896
6LU7	A_ARG_298	NH1	A_ASP_295	OD1	3.939
6LVN	B_LYS_14	NZ	B_GLU_15	OE2	3.711
6LVN	B_ARG_18	NH1	B_GLU_15	OE1	3.427
6LVN	B_LYS_24	NZ	B_GLU_21	OE1	3.825
6LVN	B_LYS_24	NZ	B_GLU_21	OE2	3.054
6LVN	C_LYS_14	NZ	C_GLU_15	OE2	2.916
6LVN	C_ARG_18	NH2	C_GLU_15	OE1	3.632
6LVN	C_ARG_18	NH2	C_GLU_15	OE2	2.854
6LVN	C_LYS_24	NZ	C_GLU_28	OE2	3.766
6LVN	C_LYS_24	NZ	D_GLU_21	OE1	3.613
6LVN	C_LYS_24	NZ	D_GLU_21	OE2	2.690
6LVN	D_ARG_18	NH2	D_GLU_15	OE1	3.866
6LVN	D_ARG_18	NH2	D_GLU_15	OE2	3.115
6LVN	D_LYS_24	NZ	C_GLU_21	OE1	3.756
6LVN	D_LYS_24	NZ	C_GLU_21	OE2	2.891
6LXT	A_LYS_921	NZ	A_GLU_918	OE2	3.662
6LXT	A_LYS_947	NZ	C_GLU_1182	OE1	2.868
6LXT	A_LYS_947	NZ	C_GLU_1182	OE2	3.665
6LXT	A_ARG_983	NH1	C_ASP_985	OD1	2.627
6LXT	A_ARG_983	NH1	C_GLU_988	OE1	3.658
6LXT	A_ARG_983	NH2	C_ASP_985	OD1	3.810
6LXT	A_ARG_1185	NH1	B_ASP_936	OD2	2.747
6LXT	A_ARG_1185	NH2	B_ASP_936	OD2	3.553
6LXT	B_LYS_947	NZ	A_GLU_1182	OE2	3.013
6LXT	B_LYS_1191	NZ	F_ASP_936	OD1	3.636
6LXT	B_LYS_1191	NZ	F_ASP_936	OD2	2.639
6LXT	C_LYS_947	NZ	B_GLU_1182	OE1	2.808
6LXT	C_ARG_983	NH1	B_GLU_988	OE2	3.205
6LXT	C_ARG_1185	NH2	A_ASP_936	OD2	3.479
6LXT	C_LYS_1191	NZ	C_GLU_1188	OE1	3.767
6LXT	D_LYS_947	NZ	F_GLU_1182	OE1	2.984
6LXT	D_LYS_947	NZ	F_GLU_1182	OE2	3.943
6LXT	D_ARG_1185	NH1	D_GLU_1188	OE2	2.798
6LXT	D_ARG_1185	NH2	D_GLU_1188	OE2	3.164
6LXT	E_LYS_921	NZ	E_GLU_1202	OE2	3.098
6LXT	E_ARG_983	NH1	D_ASP_985	OD1	3.405
6LXT	E_LYS_1191	NZ	E_GLU_1188	OE1	3.578
6LXT	F_LYS_947	NZ	E_GLU_1182	OE1	2.714
6LXT	F_LYS_947	NZ	E_GLU_1182	OE2	3.334
6LXT	F_ARG_983	NH1	F_ASP_979	OD2	3.887
6LXT	F_ARG_983	NH2	F_ASP_979	OD1	3.827

6LXT	F_ARG_983	NH2	F_ASP_979	OD2	3.090
6LXT	F_ARG_1185	NH2	D_ASP_936	OD2	3.238
6LXT	F_LYS_1191	NZ	F_GLU_1188	OE1	3.938
6VSB	A_ARG_34	NH1	A_GLU_191	OE2	3.360
6VSB	A_ARG_44	NH1	A_ASP_40	OD1	3.626
6VSB	A_ARG_44	NH1	A_ASP_40	OD2	3.805
6VSB	A_ARG_44	NH2	A_ASP_40	OD2	3.952
6VSB	A_LYS_195	NZ	A_ASP_53	OD1	3.374
6VSB	A_LYS_195	NZ	A_ASP_53	OD2	2.816
6VSB	A_LYS_206	NZ	A_GLU_224	OE2	3.715
6VSB	A_LYS_310	NZ	A_ASP_663	OD1	2.695
6VSB	A_LYS_310	NZ	A_ASP_663	OD2	2.759
6VSB	A_ARG_319	NH1	B_ASP_737	OD2	3.350
6VSB	A_ARG_319	NH1	B_ASP_745	OD1	3.737
6VSB	A_ARG_509	NH1	A_ASP_442	OD1	3.045
6VSB	A_ARG_509	NH1	A_ASP_442	OD2	3.727
6VSB	A_LYS_537	NZ	A_GLU_324	OE2	2.800
6VSB	A_LYS_557	NZ	A_ASP_568	OD1	3.297
6VSB	A_LYS_557	NZ	A_ASP_568	OD2	3.960
6VSB	A_LYS_557	NZ	A_ASP_574	OD1	2.979
6VSB	A_LYS_557	NZ	A_ASP_574	OD2	3.677
6VSB	A_ARG_567	NH1	A_ASP_571	OD1	3.120
6VSB	A_ARG_567	NH2	A_ASP_571	OD1	3.007
6VSB	A_LYS_733	NZ	A_ASP_775	OD2	2.987
6VSB	A_ARG_815	NH1	A_ASP_820	OD1	3.501
6VSB	A_ARG_995	NH1	B_ASP_994	OD2	3.301
6VSB	A_ARG_995	NH2	B_ASP_994	OD1	3.860
6VSB	A_ARG_995	NH2	B_ASP_994	OD2	3.526
6VSB	A_ARG_1019	NH1	A_GLU_773	OE1	3.451
6VSB	A_ARG_1019	NH2	A_GLU_780	OE1	3.758
6VSB	A_LYS_1028	NZ	A_GLU_725	OE1	3.331
6VSB	A_LYS_1028	NZ	A_GLU_725	OE2	2.161
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE1	3.150
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE2	2.518
6VSB	A_HIS_1064	NE2	A_GLU_725	OE1	2.548
6VSB	B_ARG_34	NH1	B_GLU_191	OE2	2.687
6VSB	B_LYS_310	NZ	B_ASP_663	OD2	3.794
6VSB	B_ARG_319	NH1	C_ASP_745	OD2	2.995
6VSB	B_ARG_319	NH2	C_ASP_745	OD2	2.259
6VSB	B_ARG_328	NH2	B_ASP_578	OD2	3.954
6VSB	B_ARG_509	NH1	B_ASP_442	OD1	3.397
6VSB	B_ARG_509	NH1	B_ASP_442	OD2	3.796
6VSB	B_LYS_535	NZ	B_GLU_554	OE2	2.837
6VSB	B_LYS_537	NZ	B_GLU_324	OE1	2.302
6VSB	B_LYS_557	NZ	B_ASP_586	OD2	3.831
6VSB	B_ARG_567	NH1	B_ASP_571	OD1	3.851
6VSB	B_ARG_567	NH1	B_ASP_571	OD2	2.777
6VSB	B_LYS_733	NZ	B_ASP_775	OD1	3.456
6VSB	B_LYS_733	NZ	B_ASP_775	OD2	2.384
6VSB	B_LYS_790	NZ	A_GLU_702	OE1	3.843
6VSB	B_LYS_811	NZ	B_GLU_868	OE2	2.474
6VSB	B_ARG_815	NH1	B_ASP_820	OD1	3.410
6VSB	B_ARG_995	NH1	C_ASP_994	OD1	3.764
6VSB	B_ARG_995	NH1	C_ASP_994	OD2	3.877
6VSB	B_ARG_995	NH2	C_ASP_994	OD1	3.426
6VSB	B_ARG_995	NH2	C_ASP_994	OD2	2.571
6VSB	B_ARG_1019	NH1	B_GLU_773	OE1	3.369
6VSB	B_ARG_1019	NH1	B_GLU_773	OE2	2.567

6VSB	B_LYS_1028	NZ	B_GLU_725	OE1	3.341
6VSB	B_LYS_1028	NZ	B_GLU_725	OE2	3.228
6VSB	B_ARG_1039	NH1	B_GLU_1031	OE1	3.814
6VSB	B_ARG_1039	NH2	C_GLU_1031	OE2	2.823
6VSB	B_HIS_1064	NE2	B_GLU_725	OE2	3.061
6VSB	C_ARG_328	NH2	C_ASP_578	OD2	3.702
6VSB	C_LYS_537	NZ	C_GLU_324	OE2	2.513
6VSB	C_LYS_557	NZ	C_ASP_568	OD1	3.721
6VSB	C_LYS_557	NZ	C_ASP_574	OD2	2.504
6VSB	C_LYS_557	NZ	C_ASP_586	OD1	3.989
6VSB	C_ARG_567	NH1	C_ASP_571	OD2	3.485
6VSB	C_ARG_567	NH2	C_ASP_571	OD2	3.926
6VSB	C_LYS_733	NZ	C_ASP_775	OD1	3.495
6VSB	C_LYS_733	NZ	C_ASP_775	OD2	2.262
6VSB	C_ARG_815	NH2	C_ASP_820	OD1	3.789
6VSB	C_ARG_995	NH2	A_ASP_994	OD1	3.992
6VSB	C_ARG_995	NH2	A_ASP_994	OD2	3.052
6VSB	C_ARG_1019	NH1	B_GLU_1017	OE2	3.054
6VSB	C_ARG_1019	NH1	C_GLU_773	OE2	2.736
6VSB	C_ARG_1019	NH2	B_GLU_1017	OE2	3.999
6VSB	C_LYS_1028	NZ	C_GLU_725	OE1	2.906
6VSB	C_LYS_1028	NZ	C_GLU_725	OE2	3.013
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE1	3.069
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE2	3.224
6VSB	C_HIS_1064	NE2	C_GLU_725	OE1	2.847

Table 1: Salt bridging networks within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
9	ARG995	ASP994
8	LYS947	GLU1182
6	ARG567	ASP571
6	LYS24	GLU21
6	LYS1028	GLU725
6	ARG1039	GLU1031
5	ARG18	GLU15
5	LYS733	ASP775
4	ARG1019	GLU773
4	ARG509	ASP442
4	ARG1185	ASP936
4	ARG131	ASP289
3	LYS310	ASP663
3	ARG983	ASP985
3	ARG815	ASP820
3	LYS537	GLU324
3	LYS557	ASP568
3	ARG319	ASP745
3	LYS1191	GLU1188
3	HIS1064	GLU725
3	LYS557	ASP574
3	ARG44	ASP40
3	ARG983	ASP979
2	ARG34	GLU191
2	ARG983	GLU988
2	ARG1185	GLU1188
2	ARG76	ASP92
2	ARG105	ASP176
2	ARG328	ASP578
2	LYS1191	ASP936
2	LYS557	ASP586
2	ARG1019	GLU1017
2	ARG40	ASP187
2	LYS195	ASP53
2	LYS14	GLU15
1	LYS790	GLU702
1	ARG1019	GLU780
1	LYS206	GLU224
1	ARG131	ASP197
1	LYS137	ASP197
1	LYS5	GLU288
1	ARG319	ASP737
1	ARG60	ASP56
1	ARG131	GLU290
1	LYS921	GLU1202
1	LYS921	GLU918
1	LYS24	GLU28
1	LYS535	GLU554
1	HIS172	GLU166
1	LYS811	GLU868
1	ARG298	ASP295

Table 2: Counting of salt bridges within the PDB entries in Table 1.

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$

Table 3: The side chain and main chain hydrogen bonding networks.In this table, the names of the PDB files correspond to the single NMR structural model split from the NMR ensemble, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB	Acceptor (A)	Donor (D)	Hydrogen (H)	D-A (Å)	H-A (Å)	$\angle ADH(°)$

Table 4: Side chain hydrogen bonding network analysis. In this table, the names of the PDB files correspond to the single NMR structural model split from the NMR ensemble, the residue naming scheme is **Chain ID_residue name_residue number**, $\angle ADH$ represents the angle formed by acceptor (A), donor (D) and hydrogen (H) ($\angle ADH$).

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LVN	C_LYS_24	NZ	D_GLU_21	OE1	3.613
6LVN	C_LYS_24	NZ	D_GLU_21	OE2	2.690
6LVN	D_LYS_24	NZ	C_GLU_21	OE1	3.756
6LVN	D_LYS_24	NZ	C_GLU_21	OE2	2.891
6LXT	A_LYS_947	NZ	C_GLU_1182	OE1	2.868
6LXT	A_LYS_947	NZ	C_GLU_1182	OE2	3.665
6LXT	A_ARG_983	NH1	C_ASP_985	OD1	2.627
6LXT	A_ARG_983	NH1	C_GLU_988	OE1	3.658
6LXT	A_ARG_983	NH2	C_ASP_985	OD1	3.810
6LXT	A_ARG_1185	NH1	B_ASP_936	OD2	2.747
6LXT	A_ARG_1185	NH2	B_ASP_936	OD2	3.553
6LXT	B_LYS_947	NZ	A_GLU_1182	OE2	3.013
6LXT	B_LYS_1191	NZ	F_ASP_936	OD1	3.636
6LXT	B_LYS_1191	NZ	F_ASP_936	OD2	2.639
6LXT	C_LYS_947	NZ	B_GLU_1182	OE1	2.808
6LXT	C_ARG_983	NH1	B_GLU_988	OE2	3.205
6LXT	C_ARG_1185	NH2	A_ASP_936	OD2	3.479
6LXT	D_LYS_947	NZ	F_GLU_1182	OE1	2.984
6LXT	D_LYS_947	NZ	F_GLU_1182	OE2	3.943
6LXT	E_ARG_983	NH1	D_ASP_985	OD1	3.405
6LXT	F_LYS_947	NZ	E_GLU_1182	OE1	2.714
6LXT	F_LYS_947	NZ	E_GLU_1182	OE2	3.334
6LXT	F_ARG_1185	NH2	D_ASP_936	OD2	3.238
6VSB	A_ARG_319	NH1	B_ASP_737	OD2	3.350
6VSB	A_ARG_319	NH1	B_ASP_745	OD1	3.737
6VSB	A_ARG_995	NH1	B_ASP_994	OD2	3.301
6VSB	A_ARG_995	NH2	B_ASP_994	OD1	3.860
6VSB	A_ARG_995	NH2	B_ASP_994	OD2	3.526
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE1	3.150
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE2	2.518
6VSB	B_ARG_319	NH1	C_ASP_745	OD2	2.995
6VSB	B_ARG_319	NH2	C_ASP_745	OD2	2.259
6VSB	B_LYS_790	NZ	A_GLU_702	OE1	3.843
6VSB	B_ARG_995	NH1	C_ASP_994	OD1	3.764
6VSB	B_ARG_995	NH1	C_ASP_994	OD2	3.877
6VSB	B_ARG_995	NH2	C_ASP_994	OD1	3.426
6VSB	B_ARG_995	NH2	C_ASP_994	OD2	2.571
6VSB	B_ARG_1039	NH2	C_GLU_1031	OE2	2.823
6VSB	C_ARG_995	NH2	A_ASP_994	OD1	3.992
6VSB	C_ARG_995	NH2	A_ASP_994	OD2	3.052
6VSB	C_ARG_1019	NH1	B_GLU_1017	OE2	3.054
6VSB	C_ARG_1019	NH2	B_GLU_1017	OE2	3.999
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE1	3.069
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE2	3.224

Table 5: Interfacial salt bridging network analysis within the PDB entries. In this table, the residue naming scheme is **Chain ID_residue name_residue number**.

Count	Residue A	Residue B
9	ARG995	ASP994
8	LYS947	GLU1182
5	ARG1039	GLU1031
4	LYS24	GLU21
4	ARG1185	ASP936
3	ARG319	ASP745
3	ARG983	ASP985
2	ARG983	GLU988
2	ARG1019	GLU1017
2	LYS1191	ASP936
1	ARG319	ASP737
1	LYS790	GLU702

Table 6: Counting of interfacial salt bridges within the PDB entries in Table 5.

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LU7	A_LYS_5	NZ	A_GLU_288	OE1	3.977
6LU7	A_ARG_40	NH2	A_ASP_187	OD1	3.040
6LU7	A_ARG_40	NH2	A_ASP_187	OD2	3.380
6LU7	A_ARG_60	NH2	A_ASP_56	OD2	3.978
6LU7	A_ARG_76	NH2	A_ASP_92	OD1	2.923
6LU7	A_ARG_76	NH2	A_ASP_92	OD2	3.767
6LU7	A_ARG_105	NH1	A_ASP_176	OD1	3.990
6LU7	A_ARG_105	NH1	A_ASP_176	OD2	2.771
6LU7	A_ARG_131	NH1	A_ASP_289	OD1	2.939
6LU7	A_ARG_131	NH1	A_ASP_289	OD2	2.873
6LU7	A_ARG_131	NH1	A_GLU_290	OE2	3.231
6LU7	A_ARG_131	NH2	A_ASP_197	OD2	3.526
6LU7	A_ARG_131	NH2	A_ASP_289	OD1	3.835
6LU7	A_ARG_131	NH2	A_ASP_289	OD2	2.581
6LU7	A_LYS_137	NZ	A_ASP_197	OD2	3.803
6LU7	A_HIS_172	NE2	A_GLU_166	OE2	2.896
6LU7	A_ARG_298	NH1	A_ASP_295	OD1	3.939

Table 7: 6LU7-specific salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LVN	B_LYS_14	NZ	B_GLU_15	OE2	3.711
6LVN	B_ARG_18	NH1	B_GLU_15	OE1	3.427
6LVN	B_LYS_24	NZ	B_GLU_21	OE1	3.825
6LVN	B_LYS_24	NZ	B_GLU_21	OE2	3.054
6LVN	C_LYS_14	NZ	C_GLU_15	OE2	2.916
6LVN	C_ARG_18	NH2	C_GLU_15	OE1	3.632
6LVN	C_ARG_18	NH2	C_GLU_15	OE2	2.854
6LVN	C_LYS_24	NZ	C_GLU_28	OE2	3.766
6LVN	C_LYS_24	NZ	D_GLU_21	OE1	3.613
6LVN	C_LYS_24	NZ	D_GLU_21	OE2	2.690
6LVN	D_ARG_18	NH2	D_GLU_15	OE1	3.866
6LVN	D_ARG_18	NH2	D_GLU_15	OE2	3.115
6LVN	D_LYS_24	NZ	C_GLU_21	OE1	3.756
6LVN	D_LYS_24	NZ	C_GLU_21	OE2	2.891

Table 8: 6LVN-specific salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LXT	A_LYS_921	NZ	A_GLU_918	OE2	3.662
6LXT	A_LYS_947	NZ	C_GLU_1182	OE1	2.868
6LXT	A_LYS_947	NZ	C_GLU_1182	OE2	3.665
6LXT	A_ARG_983	NH1	C_ASP_985	OD1	2.627
6LXT	A_ARG_983	NH1	C_GLU_988	OE1	3.658
6LXT	A_ARG_983	NH2	C_ASP_985	OD1	3.810
6LXT	A_ARG_1185	NH1	B_ASP_936	OD2	2.747
6LXT	A_ARG_1185	NH2	B_ASP_936	OD2	3.553
6LXT	B_LYS_947	NZ	A_GLU_1182	OE2	3.013
6LXT	B_LYS_1191	NZ	F_ASP_936	OD1	3.636
6LXT	B_LYS_1191	NZ	F_ASP_936	OD2	2.639
6LXT	C_LYS_947	NZ	B_GLU_1182	OE1	2.808
6LXT	C_ARG_983	NH1	B_GLU_988	OE2	3.205
6LXT	C_ARG_1185	NH2	A_ASP_936	OD2	3.479
6LXT	C_LYS_1191	NZ	C_GLU_1188	OE1	3.767
6LXT	D_LYS_947	NZ	F_GLU_1182	OE1	2.984
6LXT	D_LYS_947	NZ	F_GLU_1182	OE2	3.943
6LXT	D_ARG_1185	NH1	D_GLU_1188	OE2	2.798
6LXT	D_ARG_1185	NH2	D_GLU_1188	OE2	3.164
6LXT	E_LYS_921	NZ	E_GLU_1202	OE2	3.098
6LXT	E_ARG_983	NH1	D_ASP_985	OD1	3.405
6LXT	E_LYS_1191	NZ	E_GLU_1188	OE1	3.578
6LXT	F_LYS_947	NZ	E_GLU_1182	OE1	2.714
6LXT	F_LYS_947	NZ	E_GLU_1182	OE2	3.334
6LXT	F_ARG_983	NH1	F_ASP_979	OD2	3.887
6LXT	F_ARG_983	NH2	F_ASP_979	OD1	3.827
6LXT	F_ARG_983	NH2	F_ASP_979	OD2	3.090
6LXT	F_ARG_1185	NH2	D_ASP_936	OD2	3.238
6LXT	F_LYS_1191	NZ	F_GLU_1188	OE1	3.938

Table 9: 6LXT-specific salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6VSB	A_ARG_34	NH1	A_GLU_191	OE2	3.360
6VSB	A_ARG_44	NH1	A_ASP_40	OD1	3.626
6VSB	A_ARG_44	NH1	A_ASP_40	OD2	3.805
6VSB	A_ARG_44	NH2	A_ASP_40	OD2	3.952
6VSB	A_LYS_195	NZ	A_ASP_53	OD1	3.374
6VSB	A_LYS_195	NZ	A_ASP_53	OD2	2.816
6VSB	A_LYS_206	NZ	A_GLU_224	OE2	3.715
6VSB	A_LYS_310	NZ	A_ASP_663	OD1	2.695
6VSB	A_LYS_310	NZ	A_ASP_663	OD2	2.759
6VSB	A_ARG_319	NH1	B_ASP_737	OD2	3.350
6VSB	A_ARG_319	NH1	B_ASP_745	OD1	3.737
6VSB	A_ARG_509	NH1	A_ASP_442	OD1	3.045
6VSB	A_ARG_509	NH1	A_ASP_442	OD2	3.727
6VSB	A_LYS_537	NZ	A_GLU_324	OE2	2.800
6VSB	A_LYS_557	NZ	A_ASP_568	OD1	3.297
6VSB	A_LYS_557	NZ	A_ASP_568	OD2	3.960
6VSB	A_LYS_557	NZ	A_ASP_574	OD1	2.979
6VSB	A_LYS_557	NZ	A_ASP_574	OD2	3.677
6VSB	A_ARG_567	NH1	A_ASP_571	OD1	3.120
6VSB	A_ARG_567	NH2	A_ASP_571	OD1	3.007
6VSB	A_LYS_733	NZ	A_ASP_775	OD2	2.987
6VSB	A_ARG_815	NH1	A_ASP_820	OD1	3.501
6VSB	A_ARG_995	NH1	B_ASP_994	OD2	3.301
6VSB	A_ARG_995	NH2	B_ASP_994	OD1	3.860
6VSB	A_ARG_995	NH2	B_ASP_994	OD2	3.526
6VSB	A_ARG_1019	NH1	A_GLU_773	OE1	3.451
6VSB	A_ARG_1019	NH2	A_GLU_780	OE1	3.758
6VSB	A_LYS_1028	NZ	A_GLU_725	OE1	3.331
6VSB	A_LYS_1028	NZ	A_GLU_725	OE2	2.161
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE1	3.150
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE2	2.518
6VSB	A_HIS_1064	NE2	A_GLU_725	OE1	2.548
6VSB	B_ARG_34	NH1	B_GLU_191	OE2	2.687
6VSB	B_LYS_310	NZ	B_ASP_663	OD2	3.794
6VSB	B_ARG_319	NH1	C_ASP_745	OD2	2.995
6VSB	B_ARG_319	NH2	C_ASP_745	OD2	2.259
6VSB	B_ARG_328	NH2	B_ASP_578	OD2	3.954
6VSB	B_ARG_509	NH1	B_ASP_442	OD1	3.397
6VSB	B_ARG_509	NH1	B_ASP_442	OD2	3.796
6VSB	B_LYS_535	NZ	B_GLU_554	OE2	2.837
6VSB	B_LYS_537	NZ	B_GLU_324	OE1	2.302
6VSB	B_LYS_557	NZ	B_ASP_586	OD2	3.831
6VSB	B_ARG_567	NH1	B_ASP_571	OD1	3.851
6VSB	B_ARG_567	NH1	B_ASP_571	OD2	2.777
6VSB	B_LYS_733	NZ	B_ASP_775	OD1	3.456
6VSB	B_LYS_733	NZ	B_ASP_775	OD2	2.384
6VSB	B_LYS_790	NZ	A_GLU_702	OE1	3.843
6VSB	B_LYS_811	NZ	B_GLU_868	OE2	2.474
6VSB	B_ARG_815	NH1	B_ASP_820	OD1	3.410
6VSB	B_ARG_995	NH1	C_ASP_994	OD1	3.764
6VSB	B_ARG_995	NH1	C_ASP_994	OD2	3.877
6VSB	B_ARG_995	NH2	C_ASP_994	OD1	3.426
6VSB	B_ARG_995	NH2	C_ASP_994	OD2	2.571
6VSB	B_ARG_1019	NH1	B_GLU_773	OE1	3.369
6VSB	B_ARG_1019	NH1	B_GLU_773	OE2	2.567
6VSB	B_LYS_1028	NZ	B_GLU_725	OE1	3.341
6VSB	B_LYS_1028	NZ	B_GLU_725	OE2	3.228

6VSB	B_ARG_1039	NH1	B_GLU_1031	OE1	3.814
6VSB	B_ARG_1039	NH2	C_GLU_1031	OE2	2.823
6VSB	B_HIS_1064	NE2	B_GLU_725	OE2	3.061
6VSB	C_ARG_328	NH2	C_ASP_578	OD2	3.702
6VSB	C_LYS_537	NZ	C_GLU_324	OE2	2.513
6VSB	C_LYS_557	NZ	C_ASP_568	OD1	3.721
6VSB	C_LYS_557	NZ	C_ASP_574	OD2	2.504
6VSB	C_LYS_557	NZ	C_ASP_586	OD1	3.989
6VSB	C_ARG_567	NH1	C_ASP_571	OD2	3.485
6VSB	C_ARG_567	NH2	C_ASP_571	OD2	3.926
6VSB	C_LYS_733	NZ	C_ASP_775	OD1	3.495
6VSB	C_LYS_733	NZ	C_ASP_775	OD2	2.262
6VSB	C_ARG_815	NH2	C_ASP_820	OD1	3.789
6VSB	C_ARG_995	NH2	A_ASP_994	OD1	3.992
6VSB	C_ARG_995	NH2	A_ASP_994	OD2	3.052
6VSB	C_ARG_1019	NH1	B_GLU_1017	OE2	3.054
6VSB	C_ARG_1019	NH1	C_GLU_773	OE2	2.736
6VSB	C_ARG_1019	NH2	B_GLU_1017	OE2	3.999
6VSB	C_LYS_1028	NZ	C_GLU_725	OE1	2.906
6VSB	C_LYS_1028	NZ	C_GLU_725	OE2	3.013
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE1	3.069
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE2	3.224
6VSB	C_HIS_1064	NE2	C_GLU_725	OE1	2.847

Table 10: 6VSB-specific salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LVN	C_LYS_24	NZ	D_GLU_21	OE1	3.613
6LVN	C_LYS_24	NZ	D_GLU_21	OE2	2.690
6LVN	D_LYS_24	NZ	C_GLU_21	OE1	3.756
6LVN	D_LYS_24	NZ	C_GLU_21	OE2	2.891

Table 11: 6LVN-specific interfacial salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6LXT	A_LYS_947	NZ	C_GLU_1182	OE1	2.868
6LXT	A_LYS_947	NZ	C_GLU_1182	OE2	3.665
6LXT	A_ARG_983	NH1	C_ASP_985	OD1	2.627
6LXT	A_ARG_983	NH1	C_GLU_988	OE1	3.658
6LXT	A_ARG_983	NH2	C_ASP_985	OD1	3.810
6LXT	A_ARG_1185	NH1	B_ASP_936	OD2	2.747
6LXT	A_ARG_1185	NH2	B_ASP_936	OD2	3.553
6LXT	B_LYS_947	NZ	A_GLU_1182	OE2	3.013
6LXT	B_LYS_1191	NZ	F_ASP_936	OD1	3.636
6LXT	B_LYS_1191	NZ	F_ASP_936	OD2	2.639
6LXT	C_LYS_947	NZ	B_GLU_1182	OE1	2.808
6LXT	C_ARG_983	NH1	B_GLU_988	OE2	3.205
6LXT	C_ARG_1185	NH2	A_ASP_936	OD2	3.479
6LXT	D_LYS_947	NZ	F_GLU_1182	OE1	2.984
6LXT	D_LYS_947	NZ	F_GLU_1182	OE2	3.943
6LXT	E_ARG_983	NH1	D_ASP_985	OD1	3.405
6LXT	F_LYS_947	NZ	E_GLU_1182	OE1	2.714
6LXT	F_LYS_947	NZ	E_GLU_1182	OE2	3.334
6LXT	F_ARG_1185	NH2	D_ASP_936	OD2	3.238

Table 12: 6LXT-specific interfacial salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**

PDB ID	Residue A	Atom A	Residue B	Atom B	Distance (Å)
6VSB	A_ARG_319	NH1	B_ASP_737	OD2	3.350
6VSB	A_ARG_319	NH1	B_ASP_745	OD1	3.737
6VSB	A_ARG_995	NH1	B_ASP_994	OD2	3.301
6VSB	A_ARG_995	NH2	B_ASP_994	OD1	3.860
6VSB	A_ARG_995	NH2	B_ASP_994	OD2	3.526
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE1	3.150
6VSB	A_ARG_1039	NH2	B_GLU_1031	OE2	2.518
6VSB	B_ARG_319	NH1	C_ASP_745	OD2	2.995
6VSB	B_ARG_319	NH2	C_ASP_745	OD2	2.259
6VSB	B_LYS_790	NZ	A_GLU_702	OE1	3.843
6VSB	B_ARG_995	NH1	C_ASP_994	OD1	3.764
6VSB	B_ARG_995	NH1	C_ASP_994	OD2	3.877
6VSB	B_ARG_995	NH2	C_ASP_994	OD1	3.426
6VSB	B_ARG_995	NH2	C_ASP_994	OD2	2.571
6VSB	B_ARG_1039	NH2	C_GLU_1031	OE2	2.823
6VSB	C_ARG_995	NH2	A_ASP_994	OD1	3.992
6VSB	C_ARG_995	NH2	A_ASP_994	OD2	3.052
6VSB	C_ARG_1019	NH1	B_GLU_1017	OE2	3.054
6VSB	C_ARG_1019	NH2	B_GLU_1017	OE2	3.999
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE1	3.069
6VSB	C_ARG_1039	NH2	A_GLU_1031	OE2	3.224

Table 13: 6VSB-specific interfacial salt bridging network analysis. In this table, the residue naming scheme is **Chain ID_residue name_residue number**