Calculation of Van der Waals Energy:

$V=4.184(\sqrt{E_i+E_j})[((R_i+R_j)/r)^{12}-2((R_i+R_j)/r)^6]$ kJ/mol

V is the Van der Waals energy.
R_i+R_j are the Van der Waals radii for atoms i and j, respectively.
E is the Van der Waals well depth.
r is the distance between the atoms.

Calculation of Electrostatic Energy:

$E=4.184(332\ q_1\ q_2)/\ Dr$ kJ/mol

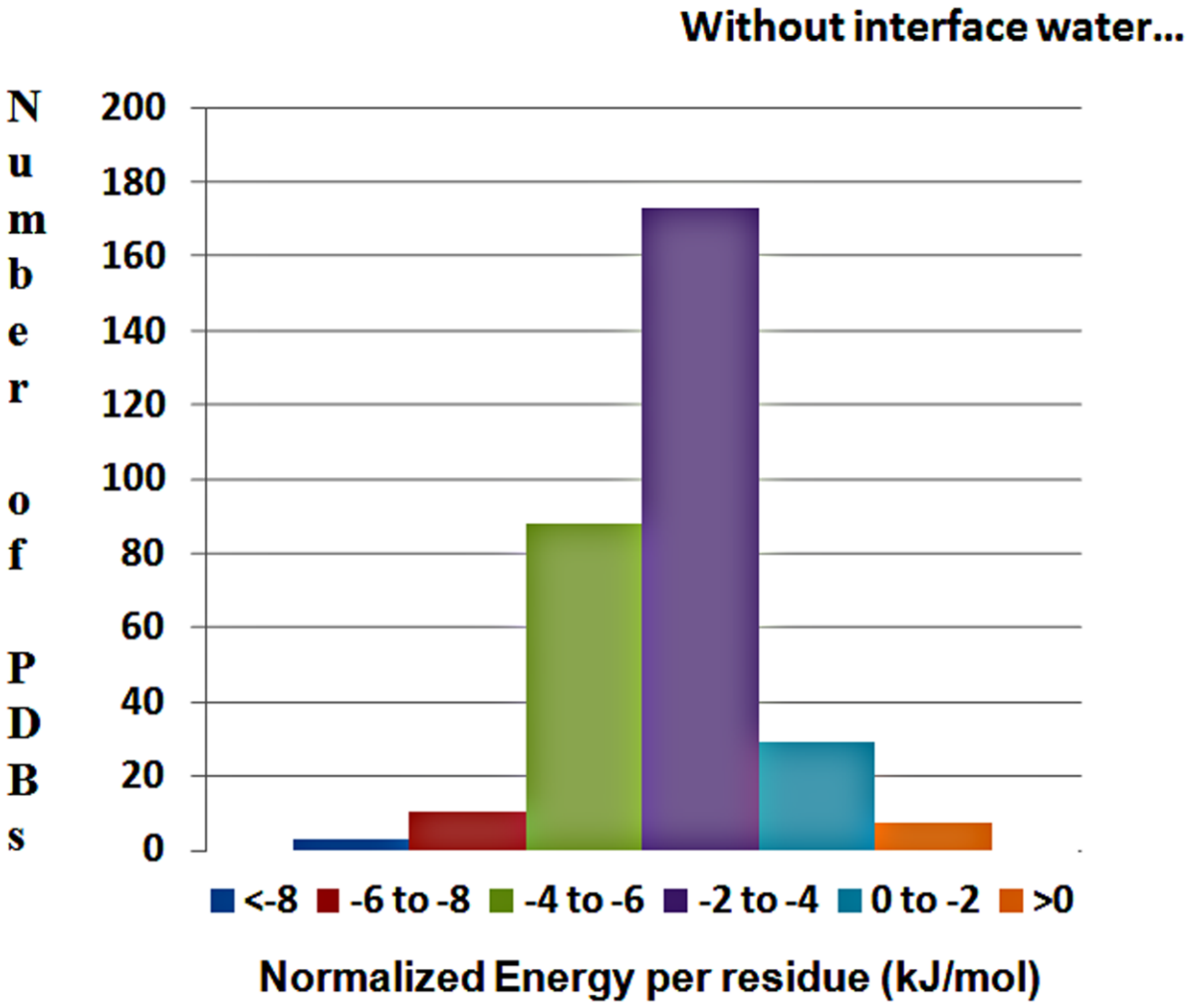
E is the electrostatic energy.
q_1 q_2 are the partial atomic charges.
r is the distance between the atoms.
D is dielectric constant of the medium; Distance dependent dilectric constant (DDD = 2r) has been used in the calculation.

Calculation of Hydrogen-Bond Energy:

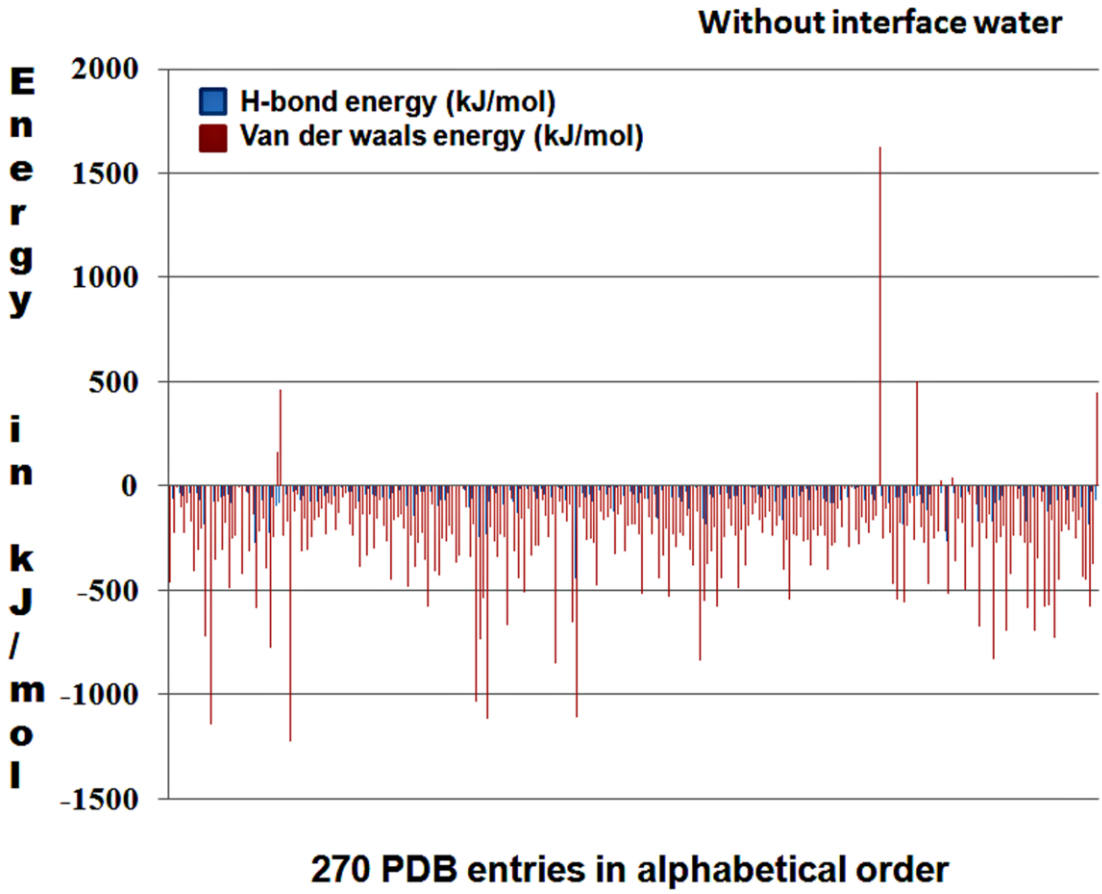
$H=0.084(1/r_{ON}+1/r_{CH}-1/r_{OH}-1/r_{CN})\ 332 * 4.184$ kJ/mol

q_1= -0.42e & q_2=0.20e when H-hond forms between two amino acids.
q_1= -0.42e & q_2=0.41e when H-hond forms between an amino acids and water and water acts as H-bond donor.
q_1= -0.82e & q_2=0.20e when H-hond forms between an amino acids and water and water acts as H-bond acceptor.

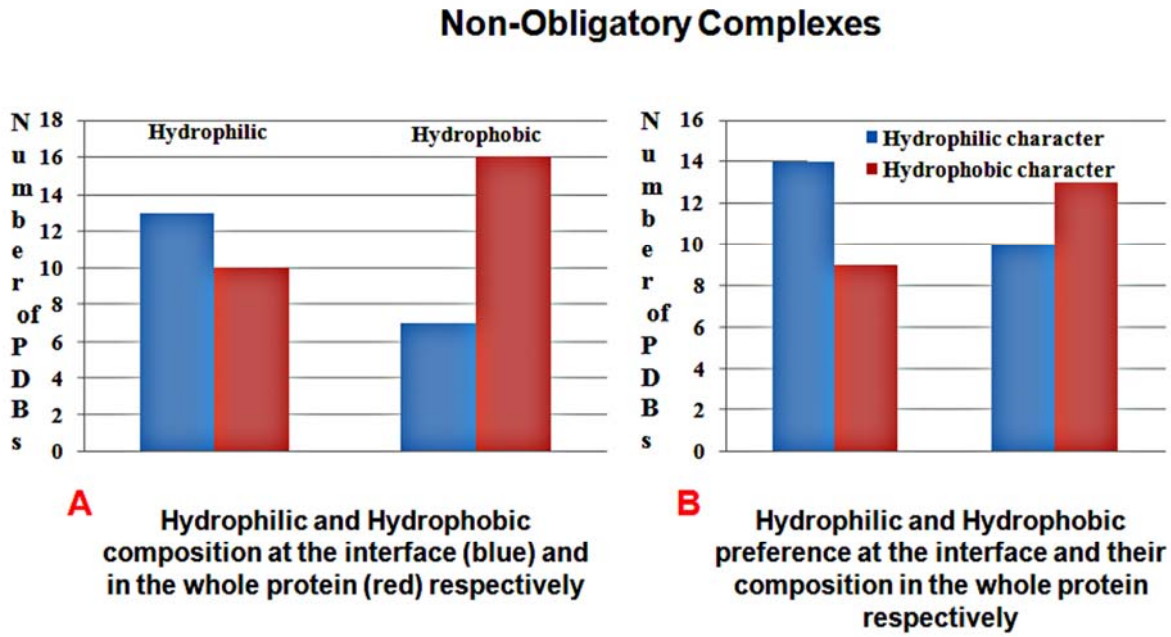
Supplementary Figure SF1: Formulae and the Description for calculating the pseudoenergies for various kinds of interactions by PPCheck server.



Supplementary Figure SF2: Histogram showing normalized energy per residue for all the protein-protein interacting complexes in the 'without-water' dataset.

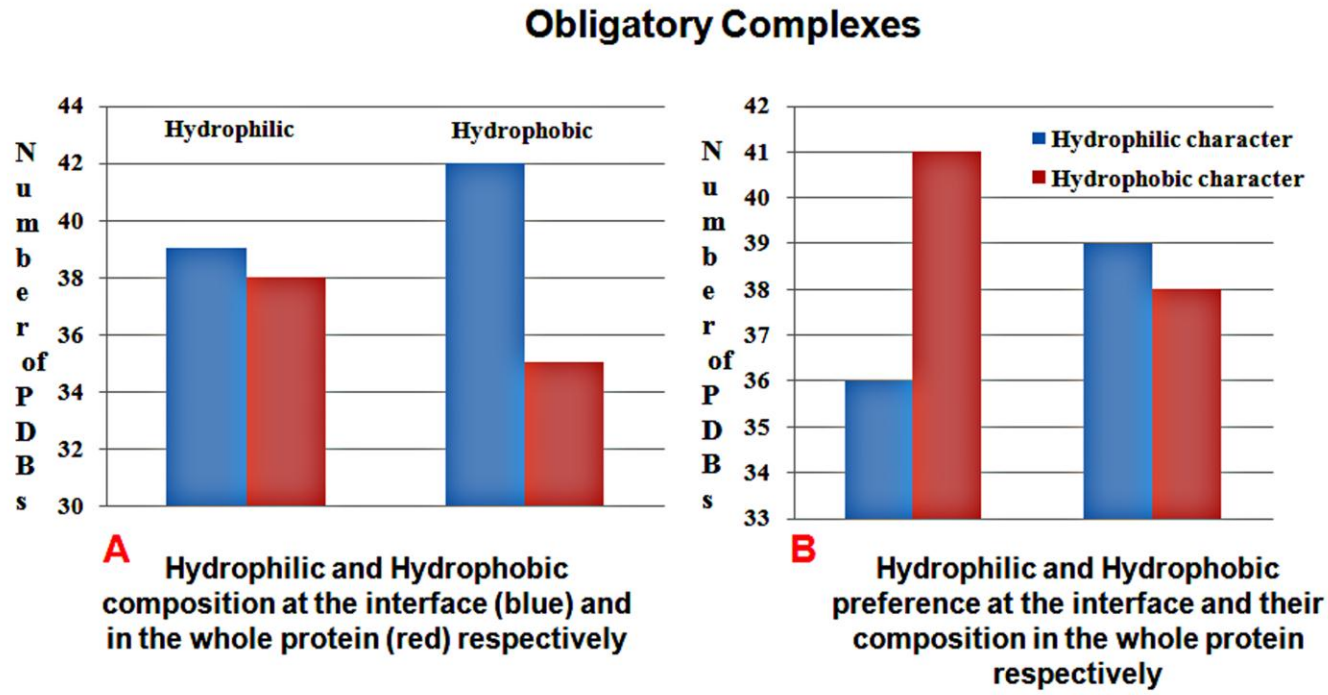


Supplementary Figure SF3: Bar graph showing relative contribution of Van der Waals interaction energy and Hydrogen bond energy towards the stability of the interacting complexes in 'without-water' dataset. Check Supplementary Table ST8 for the alphabetical names of 'without-water' dataset entries and their respective Van der Waals energy and Hydrogen-Bond energies.



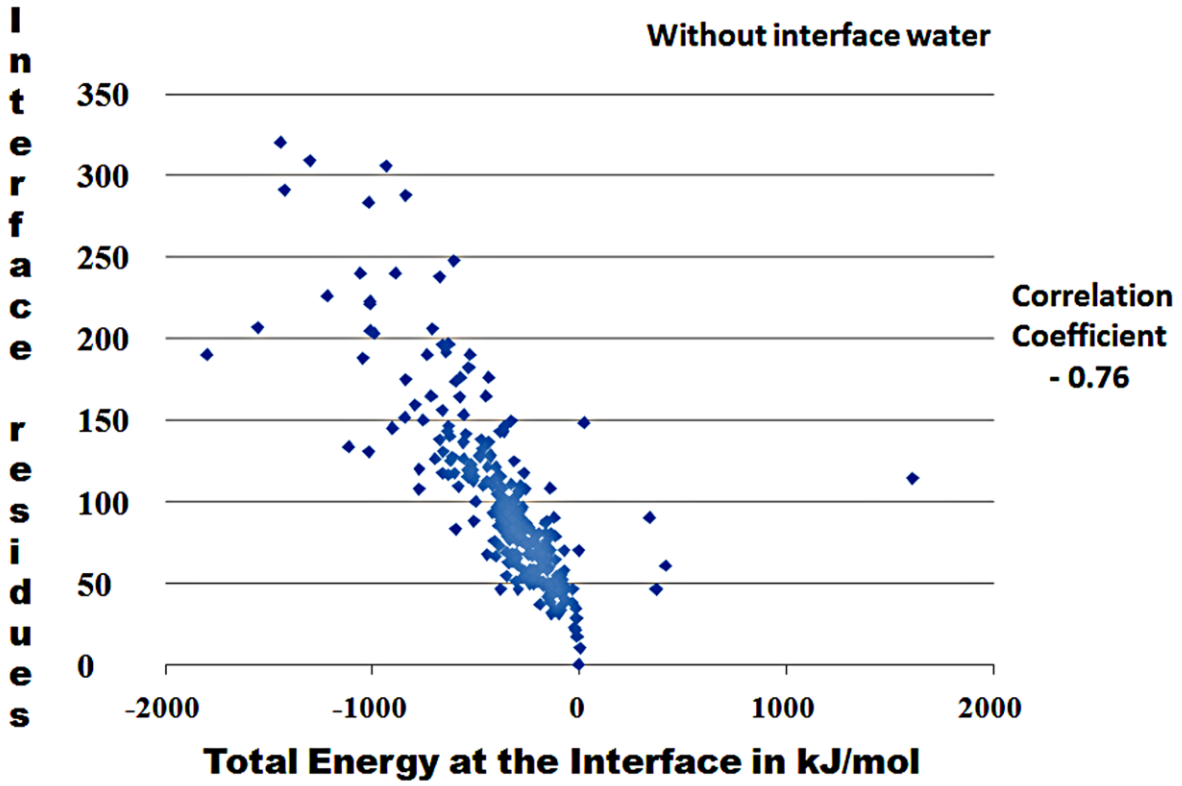
Supplementary Figure SF4(A): Relative abundance of hydrophilic residues at the interface in 13 out of 23 instances in non-obligatory complexes (blue color-1st bar) while in other 10 out of 23 instances hydrophilic residues are more in the protein as a whole (red-2nd bar). Relative abundance of hydrophobic residues at the interface in 7 out of 23 instances in non-obligatory complexes (blue color-3rd bar) while in other 16 out of 23 instances hydrophobic residues are more in the protein as a whole (red-4th bar). **Supplementary Figure SF4(B):** Relatively higher composition of hydrophilic residues at the interfaces than the hydrophobic ones in non-obligatory complexes (14 out of 23 times, blue color-1st bar) while in other 9 out of 23 instances hydrophobic residues were more than hydrophilic ones at the interface (red color-2nd bar). Relatively lower composition of hydrophilic residues in the protein as a whole (10 out of 23 cases; blue color-3rd bar), whereas higher composition of hydrophobic residues in the protein as a whole (13 out of 23 cases).

NOTE: Although there were 24 non-obligatory complexes in the selected dataset (S. De et al, 2005), for one entry (1ALK.A-C) we did not observe any interaction between the two proteins from PPCheck server.

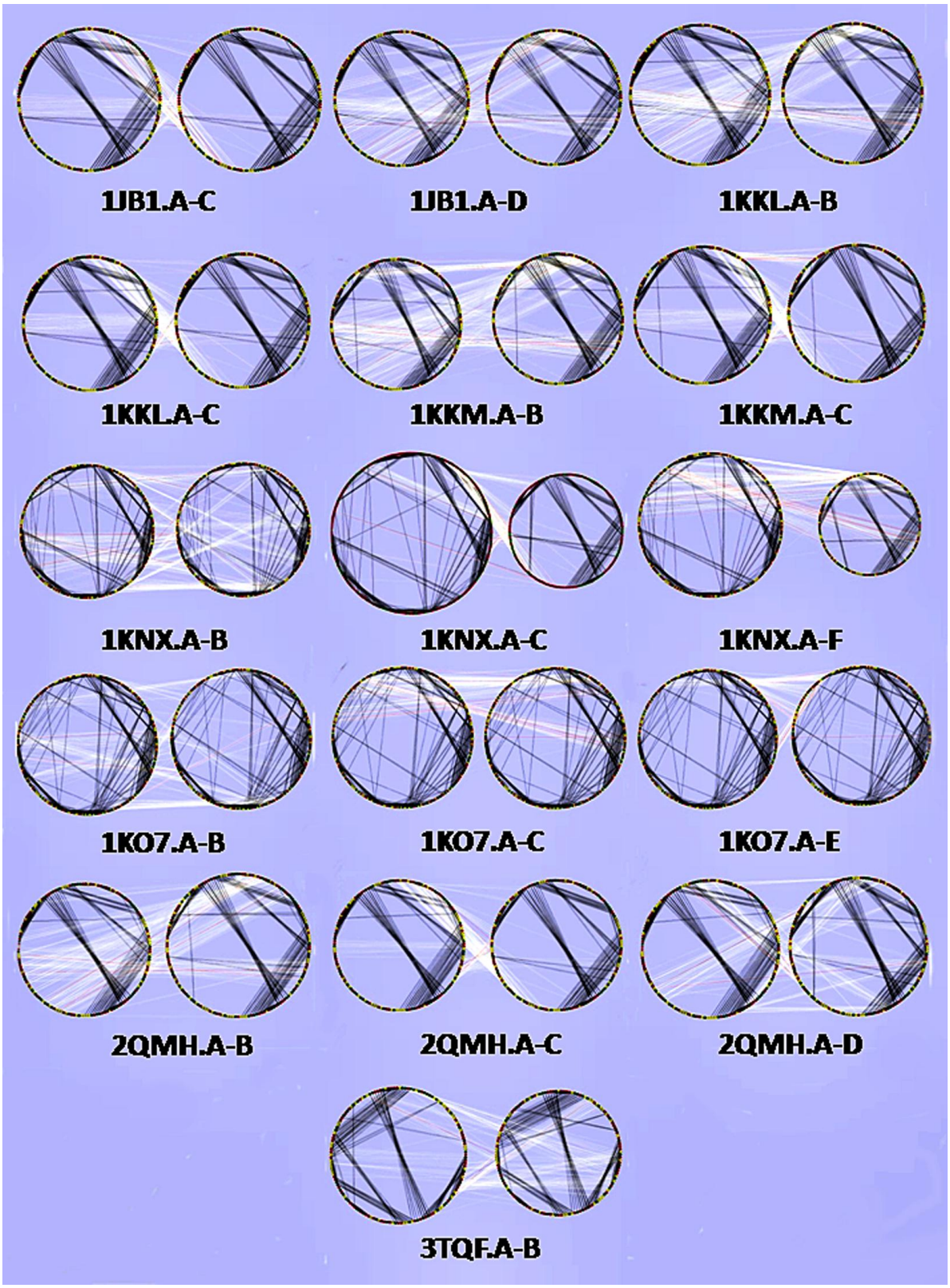


Supplementary Figure SF5(A): Relative abundance of hydrophilic residues at the interface in 39 out of 77 instances in obligatory complexes (blue color-1st bar) while in other 38 out of 77 instances hydrophilic residues are more in the protein as a whole (red-2nd bar). Relative abundance of hydrophobic residues at the interface in 42 out of 77 instances in obligatory complexes (blue color-3rd bar) while in other 35 out of 77 instances hydrophobic residues are more in the protein as a whole (red-4th bar).

Supplementary Figure SF5(B): Relatively lower composition of hydrophilic residues at the interfaces than the hydrophobic ones in obligatory complexes (36 out of 77 times, blue color-1st bar) while in other 41 out of 77 instances hydrophobic residues were more than hydrophilic ones at the interface (red color-2nd bar). Relatively higher composition of hydrophobic residues in the protein as a whole (39 out of 77 cases; blue color-3rd bar) whereas lower composition of hydrophobic residues in the protein as a whole (38 out of 77 cases).



Supplementary Figure SF6: shows Total energy v/s number of interface residues graph for the 'without-water' dataset having a correlation coefficient of -0.76.



Supplementary Figure SF7: Shows comparison of residue networks from the PASS2 domain (1KNX-A), its interacting partners (1KNX-B, 1KNX-C and 1KNX-F) along with its homologues (A chain of all other proteins shown in the figure) and their interacting partners (chain identifier following hyphen "-" in respective cases). 1KNX is a multidomain (two) protein where the two intrachain domains have some significant distance between them. This is the reason they both show two small circles with different residues contributing in intramolecular interactions. The domain which interacts with the query domain is only shown in these network representations. Also, those domains which only form intramolecular interactions have not been shown. Here, one could compare these networks just by visual inspection. Similar patterns of interactions (example, as in 1JB1.A-C and 1KKL.A-C) means, essentially they share similar interfaces.

1A2K.pdb A B 2.50	1D2Z.pdb A B 2.00	1HBN.pdb B E 1.16	1ORY.pdb A B 2.45	1STF.pdb A B 2.37	2CTS.pdb A B 2.00
1A2K.pdb A D 2.50	1DAN.pdb B C 2.00	1HFE.pdb A B 1.60	1OSP.pdb A C 1.95	1SV0.pdb B D 2.07	2GN5.pdb A B 2.30
1A2K.pdb C A 2.50	1DBF.pdb A B 1.30	1HIA.pdb B I 2.40	1OTF.pdb A C 1.90	1SVF.pdb B A 1.40	2HDH.pdb A B 2.20
1A2Y.pdb B C 1.50	1DCP.pdb A B 2.30	1HJR.pdb A C 2.50	1OTF.pdb A D 1.90	1SVF.pdb C D 1.40	2JEL.pdb B C 2.50
1A2Z.pdb A B 1.73	1DCP.pdb A C 2.30	1HWG.pdb A B 2.50	1OTF.pdb A E 1.90	1T0F.pdb A C 1.85	2KAI.pdb B I 2.50
1A2Z.pdb A D 1.73	1DCP.pdb A D 2.30	1I0H.pdb A B 1.35	1OTG.pdb A B 2.10	1T0J.pdb B C 2.00	2OHX.pdb A B 1.80
1A3C.pdb A B 1.60	1DCP.pdb A E 2.30	1ICW.pdb A B 2.01	1PGT.pdb A B 1.80	1TA3.pdb A B 1.70	2OR1.pdb L R 2.50
1A4I.pdb A B 1.50	1DEL.pdb A B 2.20	1IHF.pdb B A 2.50	1PHH.pdb A B 2.30	1TAB.pdb A B 2.30	2OZ9.pdb A B 1.65
1AA7.pdb A B 2.08	1DFJ.pdb A B 2.50	1J9L.pdb A B 1.90	1POI.pdb B A 2.50	1TAW.pdb A B 1.80	2PCC.pdb A B 2.30
1ACB.pdb A B 2.00	1DFN.pdb A B 1.90	1JBU.pdb A C 2.00	1POI.pdb B C 2.50	1TC1.pdb A B 1.41	2PCH.pdb A B 2.00
1AFW.pdb A B 1.80	1DHK.pdb A B 1.85	1JDH.pdb A B 1.90	1PP2.pdb A B 2.50	1TGS.pdb A B 1.80	2PRG.pdb B C 2.30
1AK4.pdb A D 2.36	1DKD.pdb A E 2.10	1JDP.pdb A H 2.00	1PPF.pdb A B 1.80	1TO2.pdb A B 1.30	2PTC.pdb A B 1.90
1ALK.pdb A B 2.00	1DQI.pdb A B 1.70	1JHG.pdb A B 1.30	1PYT.pdb A B 2.35	1TTW.pdb A B 2.38	2RHE.pdb A B 1.60
1AOR.pdb A B 2.30	1DQI.pdb A D 1.70	1JR8.pdb A B 1.50	1PYT.pdb B D 2.35	1TVX.pdb A B 1.75	2RUS.pdb A B 2.30
1ATL.pdb A B 1.80	1DS6.pdb A B 2.35	1JTH.pdb A B 2.00	1Q1S.pdb B C 2.30	1TVX.pdb B C 1.75	2SIC.pdb A B 1.80
1AVW.pdb A B 1.75	1DVF.pdb B D 1.90	1K9O.pdb A B 2.30	1QDL.pdb B A 2.50	1TX4.pdb A B 1.65	2SNI.pdb A B 2.10
1AY7.pdb A B 1.70	1DVJ.pdb A B 1.50	1KB5.pdb B H 2.50	1QDN.pdb A B 2.30	1TY4.pdb A B 2.20	2SOD.pdb C D 2.00
1B0N.pdb A B 1.90	1DX5.pdb I M 2.30	1KBA.pdb A B 2.30	1QFX.pdb A B 2.40	1U0S.pdb A Y 1.90	2SPC.pdb A B 1.80
1B3A.pdb A B 1.60	1DXG.pdb A B 1.80	1KSH.pdb A B 1.80	1QH4.pdb A B 1.41	1U6H.pdb A B 2.38	2TCT.pdb A B 2.10
1B55.pdb A B 2.40	1E5D.pdb A B 2.50	1KTZ.pdb A B 2.15	1QKS.pdb A B 1.28	1U8T.pdb A E 1.50	2TEC.pdb A B 1.98
1B66.pdb A B 1.90	1E96.pdb A B 2.40	1KVE.pdb A B 1.80	1QSG.pdb G E 1.75	1UAD.pdb A C 2.10	2THI.pdb A B 2.50
1B67.pdb A B 1.48	1E98.pdb A B 1.90	1KVE.pdb A C 1.80	1QSG.pdb G F 1.75	1UJZ.pdb A B 2.10	2TMK.pdb A B 2.40
1B93.pdb A B 1.90	1EAY.pdb A C 2.00	1L2I.pdb A C 1.95	1QSG.pdb G H 1.75	1US7.pdb A B 2.30	2TNF.pdb A B 1.40
1B93.pdb A C 1.90	1EFN.pdb A B 2.50	1LFD.pdb A B 2.10	1QTX.pdb A B 1.65	1USU.pdb A B 2.15	2TRC.pdb A C 2.40
1BAM.pdb A B 1.95	1EFU.pdb A B 2.50	1LQV.pdb B D 1.60	1R0R.pdb A B 1.10	1UTG.pdb A B 1.34	2TS1.pdb A B 2.30
1BCR.pdb B A 2.50	1EMV.pdb A B 1.70	1LZC.pdb A B 1.50	1R3J.pdb A C 1.90	1VF6.pdb A C 2.10	2TSC.pdb A B 1.97
1BFT.pdb A B 2.00	1EUV.pdb A B 1.60	1LYA.pdb A B 2.50	1REG.pdb A B 1.90	1VFB.pdb B C 1.80	3ENL.pdb A B 2.25
1BIF.pdb A B 2.00	1EXT.pdb A B 1.85	1M4U.pdb A L 2.42	1REW.pdb B D 1.86	1VPP.pdb A C 1.90	3FAP.pdb A B 1.85
1BJ1.pdb C D 2.40	1F37.pdb A B 2.30	1M9E.pdb B C 1.72	1RP3.pdb A B 2.30	1WDC.pdb A B 2.00	3GRS.pdb A B 1.54
1BRS.pdb A D 2.00	1F74.pdb A C 1.60	1MCT.pdb A B 1.60	1RPO.pdb A B 1.40	1WDC.pdb A C 2.00	3ICD.pdb A B 2.50
1BSR.pdb A B 1.90	1F9Z.pdb A B 1.50	1MEL.pdb A L 2.50	1RYP.pdb 1 I 1.90	1WMH.pdb A B 1.50	3NOS.pdb A B 2.40
1BTH.pdb A B 2.30	1FIN.pdb A B 2.30	1MJH.pdb A B 1.70	1RYP.pdb 1 J 1.90	1WMI.pdb A B 2.30	3PVI.pdb A B 1.59
1BXG.pdb A B 2.30	1FIP.pdb A B 1.90	1MKA.pdb A B 2.00	1RYP.pdb 1 S 1.90	1WQJ.pdb A B 1.60	3SDH.pdb A B 1.40
1C1Y.pdb A B 1.90	1FLE.pdb A B 1.90	1MLC.pdb B E 2.50	1RYP.pdb 1 T 1.90	1WWW.pdb B D 2.20	3SDP.pdb A B 2.10
1CDC.pdb A B 2.00	1FM0.pdb A B 1.45	1MSB.pdb A B 2.30	1RYP.pdb 1 Z 1.90	1XG2.pdb A B 1.90	3SGB.pdb A B 1.80
1CDT.pdb A B 2.50	1FNS.pdb B C 2.00	1MZW.pdb A B 2.00	1RYP.pdb 1 2 1.90	1YCP.pdb D E 2.50	3SSI.pdb A B 2.30
1CG2.pdb A B 2.50	1FS1.pdb A B 1.80	1NCA.pdb A B 2.50	1S6C.pdb A B 2.00	1YCS.pdb A B 2.20	3TPI.pdb A B 1.90
1CGI.pdb A B 2.30	1G6N.pdb A B 2.10	1NF3.pdb A C 2.10	1SBB.pdb A B 2.40	1YDR.pdb A B 2.20	4HTC.pdb B C 2.30
1CHO.pdb C D 1.80	1GG2.pdb A B 2.40	1NL0.pdb B C 2.20	1SBW.pdb A I 1.80	1YPI.pdb A B 1.90	4MDH.pdb A B 2.50
1COZ.pdb A B 2.00	1GL1.pdb A B 2.10	1NMB.pdb A C 2.20	1SGP.pdb A B 1.40	1YQV.pdb B C 1.70	5HVP.pdb A B 2.00
1CSE.pdb A B 1.20	1GOT.pdb A B 2.00	1OC0.pdb A B 2.28	1SHW.pdb A B 2.20	1Z7K.pdb A B 1.90	6GSV.pdb A B 1.75
1CZJ.pdb A B 2.16	1GUA.pdb A B 2.00	1OEB.pdb A D 1.76	1SKO.pdb A B 2.00	2ARC.pdb A B 1.50	6RLX.pdb A B 1.50
1CZY.pdb A D 2.00	1H2R.pdb A B 1.40	1OEY.pdb A J 2.00	1SLW.pdb A B 2.00	2BF8.pdb A B 2.30	
1D2V.pdb A B 1.75	1HBN.pdb B C 1.16	1OPH.pdb A B 2.30	1SQ2.pdb A B 1.45	2CCY.pdb A B 1.67	

Supplementary Table ST1: 238 PDBs with a total of 262 protein-protein interfaces in the dataset chosen for analysis. PDB IDs, interacting chains and resolution at which protein structure is determined have been shown consecutively.

1A2K.pdb A B 2.50	1D2Z.pdb A B 2.00	1HBN.pdb B C 1.16	1OEY.pdb A J 2.00	1SMT.pdb A B 2.20	2CCY.pdb A B 1.67
1A2K.pdb A D 2.50	1DAN.pdb B C 2.00	1HBN.pdb B E 1.16	1OPH.pdb A B 2.30	1SQ2.pdb A B 1.45	2CTS.pdb A B 2.00
1A2K.pdb C A 2.50	1DBF.pdb A B 1.30	1HFE.pdb A B 1.60	1ORY.pdb A B 2.45	1STF.pdb A B 2.37	2GN5.pdb A B 2.30
1A2Y.pdb B C 1.50	1DCP.pdb A B 2.30	1HIA.pdb B I 2.40	1OSP.pdb A C 1.95	1SV0.pdb B D 2.07	2HDH.pdb A B 2.20
1A2Z.pdb A B 1.73	1DCP.pdb A C 2.30	1HJR.pdb A C 2.50	1OTF.pdb A C 1.90	1SVF.pdb B A 1.40	2JEL.pdb B C 2.50
1A2Z.pdb A D 1.73	1DCP.pdb A D 2.30	1HWG.pdb A B 2.50	1OTF.pdb A D 1.90	1SVF.pdb C D 1.40	2KAI.pdb B I 2.50
1A3C.pdb A B 1.60	1DCP.pdb A E 2.30	1I0H.pdb A B 1.35	1OTF.pdb A E 1.90	1T0F.pdb A C 1.85	2OHX.pdb A B 1.80
1A4I.pdb A B 1.50	1DEL.pdb A B 2.20	1ICW.pdb A B 2.01	1OTG.pdb A B 2.10	1T0J.pdb B C 2.00	2OR1.pdb L R 2.50
1AA7.pdb A B 2.08	1DFJ.pdb A B 2.50	1IHF.pdb B A 2.50	1PGT.pdb A B 1.80	1TA3.pdb A B 1.70	2OZ9.pdb A B 1.65
1ACB.pdb A B 2.00	1DFN.pdb A B 1.90	1J9L.pdb A B 1.90	1PHH.pdb A B 2.30	1TAB.pdb A B 2.30	2PCC.pdb A B 2.30
1AFW.pdb A B 1.80	1DHK.pdb A B 1.85	1JBU.pdb A C 2.00	1POI.pdb B A 2.50	1TAW.pdb A B 1.80	2PCH.pdb A B 2.00
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1ALK.pdb A B 2.00	1DQI.pdb A B 1.70	1JDP.pdb A H 2.00	1PP2.pdb A B 2.50	1TGS.pdb A B 1.80	2PTC.pdb A B 1.90
1AOR.pdb A B 2.30	1DQI.pdb A D 1.70	1JHG.pdb A B 1.30	1PPF.pdb A B 1.80	1TO2.pdb A B 1.30	2RHE.pdb A B 1.60
1ATL.pdb A B 1.80	1DS6.pdb A B 2.35	1JHL.pdb B C 2.40	1PYT.pdb A B 2.35	1TTW.pdb A B 2.38	2RUS.pdb A B 2.30
1AVW.pdb A B 1.75	1DVF.pdb B D 1.90	1JR8.pdb A B 1.50	1PYT.pdb B D 2.35	1TVX.pdb A B 1.75	2SIC.pdb A B 1.80
1AY7.pdb A B 1.70	1DVJ.pdb A B 1.50	1JTH.pdb A B 2.00	1Q1S.pdb B C 2.30	1TVX.pdb B C 1.75	2SNI.pdb A B 2.10
1B0N.pdb A B 1.90	1DX5.pdb I M 2.30	1K9O.pdb A B 2.30	1QDL.pdb B A 2.50	1TX4.pdb A B 1.65	2SOD.pdb C D 2.00
1B3A.pdb A B 1.60	1DXG.pdb A B 1.80	1KB5.pdb B H 2.50	1QDN.pdb A B 2.30	1TY4.pdb A B 2.20	2SPC.pdb A B 1.80
1B55.pdb A B 2.40	1E5D.pdb A B 2.50	1KBA.pdb A B 2.30	1QFX.pdb A B 2.40	1U0S.pdb A Y 1.90	2TCT.pdb A B 2.10
1B66.pdb A B 1.90	1E96.pdb A B 2.40	1KSH.pdb A B 1.80	1QH4.pdb A B 1.41	1U6H.pdb A B 2.38	2TEC.pdb A B 1.98
1B67.pdb A B 1.48	1E98.pdb A B 1.90	1KTZ.pdb A B 2.15	1QKS.pdb A B 1.28	1U8T.pdb A E 1.50	2THI.pdb A B 2.50
1B93.pdb A B 1.90	1EAY.pdb A C 2.00	1KVE.pdb A B 1.80	1QSG.pdb G E 1.75	1UAD.pdb A C 2.10	2TMK.pdb A B 2.40
1B93.pdb A C 1.90	1EFN.pdb A B 2.50	1KVE.pdb A C 1.80	1QSG.pdb G F 1.75	1UJZ.pdb A B 2.10	2TNF.pdb A B 1.40
1BAM.pdb A B 1.95	1EFU.pdb A B 2.50	1L2I.pdb A C 1.95	1QSG.pdb G H 1.75	1US7.pdb A B 2.30	2TRC.pdb A C 2.40
1BCR.pdb B A 2.50	1EMV.pdb A B 1.70	1LFD.pdb A B 2.10	1QTX.pdb A B 1.65	1USU.pdb A B 2.15	2TS1.pdb A B 2.30
1BFT.pdb A B 2.00	1EUV.pdb A B 1.60	1LQV.pdb B D 1.60	1R0R.pdb A B 1.10	1UTG.pdb A B 1.34	2TSC.pdb A B 1.97
1BIF.pdb A B 2.00	1EXT.pdb A B 1.85	1LUC.pdb A B 1.50	1R3J.pdb A C 1.90	1VF6.pdb A C 2.10	3ENL.pdb A B 2.25
1BJ1.pdb C D 2.40	1F37.pdb A B 2.30	1LYA.pdb A B 2.50	1REG.pdb A B 1.90	1VFB.pdb B C 1.80	3FAP.pdb A B 1.85
1BMQ.pdb B A 2.50	1F74.pdb A C 1.60	1M4U.pdb A L 2.42	1REW.pdb B D 1.86	1VPP.pdb A C 1.90	3GRS.pdb A B 1.54
1BRS.pdb A D 2.00	1F9Z.pdb A B 1.50	1M9E.pdb B C 1.72	1RP3.pdb A B 2.30	1WDC.pdb A B 2.00	3ICD.pdb A B 2.50
1BSR.pdb A B 1.90	1FDL.pdb B C 2.50	1MCT.pdb A B 1.60	1RPO.pdb A B 1.40	1WDC.pdb A C 2.00	3IED.pdb A B 2.01
1BTH.pdb A B 2.30	1FIN.pdb A B 2.30	1MEL.pdb A L 2.50	1RYP.pdb 1 I 1.90	1WMH.pdb A B 1.50	3NOS.pdb A B 2.40
1BXG.pdb A B 2.30	1FIP.pdb A B 1.90	1MJH.pdb A B 1.70	1RYP.pdb 1 J 1.90	1WMI.pdb A B 2.30	3PVI.pdb A B 1.59
1C1Y.pdb A B 1.90	1FLE.pdb A B 1.90	1MKA.pdb A B 2.00	1RYP.pdb 1 S 1.90	1WQJ.pdb A B 1.60	3SDH.pdb A B 1.40
1CDC.pdb A B 2.00	1FM0.pdb A B 1.45	1MLC.pdb B E 2.50	1RYP.pdb 1 T 1.90	1WWW.pdb B D 2.20	3SDP.pdb A B 2.10
1CDT.pdb A B 2.50	1FNS.pdb B C 2.00	1MSB.pdb A B 2.30	1RYP.pdb 1 Z 1.90	1XG2.pdb A B 1.90	3SGB.pdb A B 1.80
1CG2.pdb A B 2.50	1FS1.pdb A B 1.80	1MZW.pdb A B 2.00	1RYP.pdb 1 2 1.90	1YCP.pdb D E 2.50	3SSI.pdb A B 2.30
1CGI.pdb A B 2.30	1G6N.pdb A B 2.10	1NCA.pdb A B 2.50	1S6C.pdb A B 2.00	1YCS.pdb A B 2.20	3TPI.pdb A B 1.90
1CHO.pdb C D 1.80	1GG2.pdb A B 2.40	1NF3.pdb A C 2.10	1SBB.pdb A B 2.40	1YDR.pdb A B 2.20	4CPA.pdb A I 2.50
1COZ.pdb A B 2.00	1GL1.pdb A B 2.10	1NL0.pdb B C 2.20	1SBW.pdb A I 1.80	1YPI.pdb A B 1.90	4HTC.pdb B C 2.30
1CSE.pdb A B 1.20	1GLN.pdb A B 2.50	1NMB.pdb A C 2.20	1SGP.pdb A B 1.40	1YQV.pdb B C 1.70	4MDH.pdb A B 2.50
1CZJ.pdb A B 2.16	1GOT.pdb A B 2.00	1NW9.pdb A B 2.40	1SHW.pdb A B 2.20	1Z7K.pdb A B 1.90	5HVP.pdb A B 2.00
1CZY.pdb A D 2.00	1GUA.pdb A B 2.00	1OC0.pdb A B 2.28	1SKO.pdb A B 2.00	2ARC.pdb A B 1.50	6GSV.pdb A B 1.75
1D2V.pdb A B 1.75	1H2R.pdb A B 1.40	1OEB.pdb A D 1.76	1SLW.pdb A B 2.00	2BF8.pdb A B 2.30	6RLX.pdb A B 1.50

Supplementary Table ST2: 'Without-water' dataset showing 246 PDBs with a total of 270 protein-protein interfaces. PDB IDs, interacting chains and resolution at which protein structure is determined have been shown consecutively.

Supplementary Table ST3: An example of 'with-water' dataset showing Hydrogen-bond interactions (and the energy associated with them) between two amino acids and between an amino acid and a water molecule from two chains (A and B) of the PDB complex 1A2Z as obtained by PPCheck server. For the 'without-water' dataset, if the same PDDB file 1A2Z is used, then the user will not find any amino acid-water (HOH) interaction in this output; but all the other hydrogen bonds between amino acids will be reported.

****

81	ARG	A	645	NH1	101	ASP	B	2714	OD1	SS	2.749874	-3.779980
81	ARG	A	646	NH2	101	ASP	B	2715	OD2	SS	2.984765	-4.589398
88	ASP	A	696	OD2	690	HOH	B	3725	O	SB	2.932431	-9.027351
101	ASP	A	795	O	217	LYS	B	3633	NZ	BS	3.214224	-2.427427
101	ASP	A	798	OD1	81	ARG	B	2557	NH1	SS	2.698749	-2.889332
101	ASP	A	798	OD1	81	ARG	B	2558	NH2	SS	2.708259	-2.899886
101	ASP	A	799	OD2	81	ARG	B	2558	NH2	SS	3.086039	-5.945856
119	ARG	A	938	NE	101	ASP	B	2715	OD2	SS	2.897908	-10.109437
119	ARG	A	941	NH2	88	ASP	B	2611	OD1	SS	3.110210	-3.830133
119	ARG	A	941	NH2	88	ASP	B	2612	OD2	SS	2.725658	-3.141261
219	PRO	A	1729	O	90	ARG	B	2627	NH1	BS	3.060733	-6.260595
629	HOH	A	1749	O	111	ALA	A	872	N	HAc	3.067256	-13.978197
629	HOH	A	1749	O	111	ALA	B	2788	N	HAc	3.085017	-7.282054
629	HOH	A	1749	O	111	ALA	B	2791	O	HDr	3.531155	-10.753328

634 HOH A 1754 O 88 ASP B 2612 OD2 BS 2.542550 -4.160254

634 HOH A 1754 O 119 ARG A 941 NH2 HAc 3.550473 -8.006944

634 HOH A 1754 O 140 THR B 3006 OG1 HAc 3.969184 -4.004785

634 HOH A 1754 O 88 ASP B 2612 OD2 HDr 2.542550 -8.528521

669 HOH A 1789 O 88 ASP B 2612 OD2 BS 3.232564 -5.951417

669 HOH A 1789 O 220 LEU A 1733 N HAc 2.933532 -20.489611

669 HOH A 1789 O 119 ARG A 940 NH1 HAc 3.184261 -8.277882

669 HOH A 1789 O 88 ASP B 2612 OD2 HDr 3.232564 -12.200405

684 HOH A 1804 O 136 TYR B 2985 OH HAc 2.688758 -21.028238

684 HOH A 1804 O 119 ARG B 2856 NH1 HAc 3.735155 -4.594191

684 HOH A 1804 O 88 ASP A 696 OD2 HDr 2.557697 -31.556991

707 HOH A 1827 O 119 ARG B 2857 NH2 HAc 3.506070 -11.141111

707 HOH A 1827 O 220 LEU B 3649 N HAc 4.121041 -2.522195

707 HOH A 1827 O 89 ALA A 700 O HDr 2.888572 -20.787190

707 HOH A 1827 O 88 ASP A 696 OD2 HDr 3.061540 -6.897937

712 HOH A 1832 O 136 TYR A 1061 O HDr 2.651667 -31.737670

712 HOH A 1832 O 136 TYR B 2977 O HDr 2.789932 -27.370955

715 HOH A 1835 O 184 LYS B 3373 NZ HAc 2.777740 -20.985041

715 HOH A 1835 O 182 LEU A 1440 O HDr 2.762986 -26.903649

638 HOH B 3673 O 90 ARG B 2618 N HAc 4.182549 -4.957550

638 HOH B 3673 O 119 ARG A 941 NH2 HAc 3.935949 -4.149879

638 HOH B 3673 O 89 ALA B 2616 O HDr 2.799546 -21.861855

638 HOH B 3673 O 88 ASP B 2612 OD2 HDr 3.279862 -3.996503

690 HOH B 3725 O 220 LEU B 3649 N HAc 3.685853 -6.510361

690 HOH B 3725 O 119 ARG B 2857 NH2 HAc 3.824664 -4.941638

690 HOH B 3725 O 88 ASP A 696 OD2 HDr 2.932431 -18.506070

720 HOH B 3755 O 184 LYS A 1457 NZ HAc 2.680991 -24.423848

720 HOH B 3755 O 182 LEU B 3356 O HDr 2.664366 -30.389843

726 HOH B 3761 O 81 ARG A 646 NH2 HAc 4.107212 -3.645829

726 HOH B 3761 O 101 ASP B 2715 OD2 HDr 2.411605 -42.521836

726 HOH B 3761 O 216 ILE A 1704 O HDr 3.066627 -19.464510

****

Supplementary Table ST4: An example showing favorable electrostatic interactions (between positively and negatively charged amino acids) between amino-acids (and the energy associated with them) from two chains (A and B) of the PDB complex 1A2Z as obtained from PPCheck server.

****

81	ARG	A	640	CB	88 ASP B 2609 CB 9.6076 -11.74094
81	ARG	A	640	CB	101 ASP B 2712 CB 9.6761 -42.07587
88	ASP	A	693	CB	81 ARG B 2552 CB 9.6157 -9.96299
88	ASP	A	693	CB	119 ARG B 2851 CB 9.6290 -32.47680
88	ASP	A	693	CB	217 LYS B 3629 CB 9.3098 -2.18321
101	ASP	A	796	CB	81 ARG B 2552 CB 9.6695 -49.07927
101	ASP	A	796	CB	119 ARG B 2851 CB 7.5749 -21.24675
101	ASP	A	796	CB	217 LYS B 3629 CB 5.3980 -7.63089
102	GLU	A	804	CB	217 LYS B 3629 CB 9.4366 -2.40264
119	ARG	A	935	CB	88 ASP B 2609 CB 9.8218 -35.98941
119	ARG	A	935	CB	101 ASP B 2712 CB 7.8797 -29.02107
217	LYS	A	1713	CB	101 ASP B 2712 CB 6.4614 -1.11615

****

Supplementary Table ST5: An example showing unfavorable electrostatic interactions (between either two positively charged or between two negatively charged amino-acids) between amino acids (and the energy associated with them) from 2 chains (A and B) of the PDB complex 1A2Z, as obtained from PPCheck server.

****

101 ASP A	796 CB	215 ASP B	3613 CB	8.3069	8.21489
184 LYS A	1453 CB	184 LYS B	3369 CB	9.2063	1.99242
215 ASP A	1697 CB	101 ASP B	2712 CB	7.8972	9.06523

****

Supplementary Table ST6: An example showing Van der waals interactions (and the energy associated with them) between atoms from two amino acids from two chains (A and B) of the PDB complex 1A2Z, as obtained from PPCheck server.

****

81	ARG	A	1305	CA	86	ILE	B	5453	HD11	6.48186	-0.0032747
81	ARG	A	1305	CA	86	ILE	B	5455	HD13	6.76539	-0.00253518
81	ARG	A	1305	CA	110	LEU	B	5820	HD21	6.7806	-0.00250136
81	ARG	A	1306	C	86	ILE	B	5444	CD1	6.66005	-0.0176178
81	ARG	A	1306	C	86	ILE	B	5453	HD11	5.94845	-0.00546724
81	ARG	A	1306	C	86	ILE	B	5454	HD12	6.60274	-0.00293231
81	ARG	A	1306	C	86	ILE	B	5455	HD13	6.60503	-0.00292622
81	ARG	A	1306	C	110	LEU	B	5811	CD2	6.5056	-0.0202538
81	ARG	A	1306	C	110	LEU	B	5817	HD11	6.57597	-0.00300438
81	ARG	A	1306	C	110	LEU	B	5820	HD21	5.44787	-0.00922117
81	ARG	A	1306	C	110	LEU	B	5821	HD22	6.80501	-0.00244816
81	ARG	A	1306	C	110	LEU	B	5822	HD23	6.80815	-0.00244141
81	ARG	A	1307	O	86	ILE	B	5444	CD1	6.27556	-0.0186988
81	ARG	A	1307	O	86	ILE	B	5453	HD11	5.42406	-0.0063812
81	ARG	A	1307	O	86	ILE	B	5454	HD12	6.37311	-0.00243434
81	ARG	A	1307	O	86	ILE	B	5455	HD13	6.29708	-0.00261566
81	ARG	A	1307	O	110	LEU	B	5809	CG	6.73687	-0.0122485
81	ARG	A	1307	O	110	LEU	B	5810	CD1	6.6822	-0.012859

81 ARG A 1307 O 110 LEU B 5811 CD2 5.6518 -0.0348194

81 ARG A 1307 O 110 LEU B 5816 HG 6.87525 -0.0015457

****

Supplementary Table ST7: The contribution of hydrogen bond energy and Van der Waals energy to the total energy for all entries in the dataset.

PDB_ID (Interacting Chains)	Hydrogen-Bond Energy	Van der Waals Energy
1A2K.pdb (A-B)	-357.849239	-873.607019
1A2K.pdb (A-D)	-304.696362	-544.917682
1A2K.pdb (C-A)	0	-7.99401
1A2Y.pdb (B-C)	-368.601714	-458.002334
1A2Z.pdb (A-B)	-559.540616	-1009.247066
1A2Z.pdb (A-D)	-44.430637	-125.893837
1A3C.pdb (A-B)	-34.862977	-165.494297
1A4I.pdb (A-B)	-837.610532	-1236.231332
1AA7.pdb (A-B)	-294.936985	-589.086255
1ACB.pdb (A-B)	-145.818703	-367.157623
1AFW.pdb (A-B)	-1748.076349	-2447.032929
1AK4.pdb (A-C)	0	0
1ALK.pdb (A-B)	-164.075265	-1444.958855
1AOR.pdb (A-B)	-495.309143	-925.985253
1ATL.pdb (A-B)	-345.553777	-418.529647
1AVW.pdb (A-B)	-189.693283	-550.720013
1AY7.pdb (A-B)	-444.787613	-716.610133
1B0N.pdb (A-B)	-324.775401	-883.526441
1B3A.pdb (A-B)	-679.960383	-948.604893
1B55.pdb (A-B)	-415.930166	-662.220356
1B66.pdb (A-B)	-23.37649	-30.25522
1B67.pdb (A-B)	-186.806242	-652.369312
1B93.pdb (A-B)	-28.834002	-53.453362
1B93.pdb (A-C)	-247.389354	-606.451284
1BAM.pdb (A-B)	0	-197.68285
1BCR.pdb (B-A)	-1498.349104	-2061.407004
1BFT.pdb (A-B)	-64.198907	-361.362717
1BIF.pdb (A-B)	-67.565202	-358.335442
1BJ1.pdb (C-D)	-279.688013	-717.124153
1BRS.pdb (A-D)	-625.16209	-980.637
1BSR.pdb (A-B)	-791.959222	-673.003592
1BTH.pdb (A-B)	-250.227808	169.819502
1BXG.pdb (A-B)	-363.305094	-668.539914
1C1Y.pdb (A-B)	-361.532653	-617.980673
1CDC.pdb (A-B)	-1277.646318	-2480.783408
1CDT.pdb (A-B)	-57.505316	-177.596316
1CG2.pdb (A-B)	-80.239687	-135.634877
1CGI.pdb (A-B)	-95.441015	-424.014375
1CHO.pdb (C-D)	-151.052859	-306.161859
1COZ.pdb (A-B)	-290.002746	-589.787726
1CSE.pdb (A-B)	-448.693309	-703.561989
1CZJ.pdb (A-B)	-44.243303	-204.005223
1CZY.pdb (A-D)	-316.875657	-459.670827
1D2V.pdb (A-B)	-489.626655	-649.222415
1D2Z.pdb (A-B)	-411.414308	-653.800728
1DAN.pdb (B-C)	-191.084688	-292.962528
1DBF.pdb (A-B)	-614.082313	-708.164873
1DCP.pdb (A-B)	-395.754696	-594.116286
1DCP.pdb (A-C)	-177.319663	-286.224353
1DCP.pdb (A-D)	-115.598403	-206.225183
1DCP.pdb (A-E)	-57.09732	-94.69483

1DEL.pdb (A-B)	-162.948465	-367.311505
1DFJ.pdb (A-B)	-28.823078	-356.626878
1DFN.pdb (A-B)	-54.968686	-163.976686
1DHK.pdb (A-B)	-571.572218	-943.620918
1DKD.pdb (A-E)	-14.049294	-141.896984
1DQI.pdb (A-B)	-798.416507	-1130.956157
1DQI.pdb (A-D)	-632.691913	-767.865333
1DS6.pdb (A-B)	-381.596856	-716.752546
1DVF.pdb (B-D)	-253.914835	-429.842445
1DVJ.pdb (A-B)	-327.91941	-374.27617
1DX5.pdb (I-M)	-561.009457	-817.894677
1DXG.pdb (A-B)	-330.767736	-602.782496
1E5D.pdb (A-B)	-954.695698	-1417.194498
1E96.pdb (A-B)	-229.758568	-404.906098
1E98.pdb (A-B)	0	-140.18966
1EAY.pdb (A-C)	-44.173752	-203.539202
1EFN.pdb (A-B)	-145.036484	-392.285414
1EFU.pdb (A-B)	-661.373476	-1223.746256
1EMV.pdb (A-B)	-141.80886	-444.60343
1EUV.pdb (A-B)	-866.774176	-1491.971496
1EXT.pdb (A-B)	-974.155884	-1256.671014
1F37.pdb (A-B)	-196.996841	-425.055231
1F74.pdb (A-C)	-483.265916	-990.553966
1F9Z.pdb (A-B)	-1028.755273	-1681.131313
1FIN.pdb (A-B)	-418.947483	-879.519223
1FIP.pdb (A-B)	-397.972495	-905.188485
1FLE.pdb (A-B)	-430.353724	-735.972914
1FM0.pdb (A-B)	-531.424237	-820.844077
1FNS.pdb (B-C)	-308.162516	-548.805186
1FS1.pdb (A-B)	-201.179592	-441.080092
1G6N.pdb (A-B)	-123.322095	-508.446005
1GG2.pdb (A-B)	-268.313504	-672.221664
1GL1.pdb (A-B)	-112.42569	-127.10349
1GOT.pdb (A-B)	-856.514256	-1218.440656
1GUA.pdb (A-B)	-336.664406	-607.175346
1H2R.pdb (A-B)	-2351.321122	-3472.531692
1HBN.pdb (B-C)	-1169.741781	-2142.838151
1HBN.pdb (B-E)	-1699.162702	-2213.685782
1HFE.pdb (A-B)	-1690.572553	-2880.004413
1HIA.pdb (B-I)	-202.509536	-456.564286
1HJR.pdb (A-C)	-112.785767	-367.903077
1HWG.pdb (A-B)	-271.267588	-683.078288
1I0H.pdb (A-B)	-422.774472	-699.594432
1ICW.pdb (A-B)	-317.894074	-616.047474
1IHF.pdb (B-A)	-1028.903261	-1742.467271
1J9L.pdb (A-B)	-254.620691	-315.401391
1JBU.pdb (A-C)	-440.38926	-808.56322
1JDH.pdb (A-B)	-966.787741	-1547.192551
1JDP.pdb (A-H)	-203.195164	-397.124054
1JHG.pdb (A-B)	-672.954828	-1266.126198
1JR8.pdb (A-B)	-464.693323	-830.780853
1JTH.pdb (A-B)	-27.224083	-370.523343
1K9O.pdb (A-B)	-231.680128	-531.597158
1KB5.pdb (B-H)	-92.254516	-162.599506
1KBA.pdb (A-B)	-278.254041	-418.969041
1KSH.pdb (A-B)	-573.83646	-831.08919
1KTZ.pdb (A-B)	-581.867049	-762.209099

1KVE.pdb (A-B)	-817.697438	-1674.299288
1KVE.pdb (A-C)	-346.043122	-424.133522
1L2I.pdb (A-C)	-105.259704	-235.949744
1LFD.pdb (A-B)	-326.224768	-554.612598
1LQV.pdb (B-D)	-96.200663	-183.019063
1LUC.pdb (A-B)	-1591.829672	-2252.728852
1LYA.pdb (A-B)	-717.829182	-1827.757032
1M4U.pdb (A-L)	-150.017942	-251.412942
1M9E.pdb (B-C)	-312.108168	-468.226168
1MCT.pdb (A-B)	-361.798828	-667.879608
1MEL.pdb (A-L)	-43.117137	-287.230847
1MJH.pdb (A-B)	-441.888869	-714.984129
1MKA.pdb (A-B)	-963.400669	-1548.096429
1MLC.pdb (B-E)	-121.043357	-328.698697
1MSB.pdb (A-B)	-52.222091	-212.788011
1MZW.pdb (A-B)	-454.758938	-615.849648
1NCA.pdb (A-B)	-3.402811	-105.251021
1NF3.pdb (A-C)	-646.068039	-980.921579
1NL0.pdb (B-C)	-202.879667	-336.960397
1NMB.pdb (A-C)	-45.902415	-138.046455
1OC0.pdb (A-B)	-201.2602	-451.39942
1OEB.pdb (A-D)	-368.622501	-635.149751
1OEY.pdb (A-J)	-412.583004	-678.953074
1OPH.pdb (A-B)	-328.561635	-604.695645
1ORY.pdb (A-B)	-261.22928	-845.49114
1OSP.pdb (A-C)	-13.425325	-80.565475
1OTF.pdb (A-C)	-59.793689	-235.007439
1OTF.pdb (A-D)	-68.795105	-304.560795
1OTF.pdb (A-E)	-50.421502	-215.890832
1OTG.pdb (A-B)	-695.425404	-1169.389404
1PGT.pdb (A-B)	-900.325597	-1312.361647
1PHH.pdb (A-B)	-24.877955	-237.627955
1POI.pdb (B-A)	-737.681472	-1278.317152
1POI.pdb (B-C)	-193.065723	-492.582893
1PP2.pdb (A-B)	-352.094669	-702.044239
1PPF.pdb (A-B)	-390.924023	-623.672083
1PYT.pdb (A-B)	-329.189234	-656.606994
1PYT.pdb (B-D)	-155.597949	-296.012949
1Q1S.pdb (B-C)	-418.711621	-730.126451
1QDL.pdb (B-A)	-129.066838	-510.849448
1QDN.pdb (A-B)	-423.894892	-579.590802
1QFX.pdb (A-B)	-1738.326431	-2640.313551
1QH4.pdb (A-B)	-1873.741736	-2548.793076
1QKS.pdb (A-B)	-1861.665779	-2253.464519
1QSG.pdb (G-E)	-680.694476	-1008.026086
1QSG.pdb (G-F)	-159.451131	-341.812121
1QSG.pdb (G-H)	-622.108086	-1328.226376
1QTX.pdb (A-B)	-572.85056	-1190.5469
1R0R.pdb (A-B)	-564.703124	-819.759424
1R3J.pdb (A-C)	-281.864499	-436.929159
1REG.pdb (A-B)	-207.065249	-448.210379
1REW.pdb (B-D)	-557.80896	-818.04922
1RP3.pdb (A-B)	-145.427796	-667.769826
1RPO.pdb (A-B)	0	-293.42267
1RYP.pdb (1-I)	-598.007345	-1048.850965
1RYP.pdb (1-J)	-207.932592	-421.883692
1RYP.pdb (1-S)	-341.223555	-515.089715

1RYP.pdb (1-T)	-52.033109	-162.117179
1RYP.pdb (1-Z)	-237.445843	-452.678013
1RYP.pdb (1-2)	-794.110012	-1045.751012
1S6C.pdb (A-B)	-63.788007	-211.789007
1SBB.pdb (A-B)	-145.519209	-273.544539
1SBW.pdb (A-I)	-606.728981	-862.142181
1SGP.pdb (A-B)	-181.889062	-380.256052
1SHW.pdb (A-B)	-151.90272	-302.79537
1SKO.pdb (A-B)	-545.296551	-959.575581
1SLW.pdb (A-B)	-78.061149	-301.506869
1SQ2.pdb (A-B)	-619.513326	-913.835366
1STF.pdb (A-B)	-286.798309	-523.946309
1SV0.pdb (B-D)	-160.214231	-381.947421
1SVF.pdb (B-A)	-185.481324	-455.763154
1SVF.pdb (C-D)	-209.164152	-444.684912
1T0F.pdb (A-C)	-515.972008	-959.595988
1T0J.pdb (B-C)	-13.090567	-232.060217
1TA3.pdb (A-B)	-1162.140106	-1411.978556
1TAB.pdb (A-B)	-203.814863	-408.955503
1TAW.pdb (A-B)	-171.75578	-452.31743
1TC1.pdb (A-B)	-832.962264	-1305.674064
1TGS.pdb (A-B)	-420.656622	-720.174002
1TO2.pdb (A-B)	-666.870096	-976.906126
1TTW.pdb (A-B)	0	-112.09
1TVX.pdb (A-B)	-393.302921	-577.256381
1TVX.pdb (B-C)	-194.77552	-208.91162
1TX4.pdb (A-B)	-822.566878	-1210.538268
1TY4.pdb (A-B)	0	7.204913
1U0S.pdb (A-Y)	-1590.000488	-1818.325238
1U6H.pdb (A-B)	-5.761313	-289.539093
1U8T.pdb (A-E)	-144.826431	-311.537111
1UAD.pdb (A-C)	-287.329618	-518.549198
1UJZ.pdb (A-B)	-306.754075	-624.976615
1US7.pdb (A-B)	-443.909129	-608.813809
1USU.pdb (A-B)	-522.564478	-812.057978
1UTG.pdb (A-B)	0	1609.85559
1VF6.pdb (A-C)	-75.184395	-405.403455
1VFB.pdb (B-C)	-356.479179	-447.832119
1VPP.pdb (A-C)	-184.706742	-477.228232
1WDC.pdb (A-B)	-239.573459	-809.583159
1WDC.pdb (A-C)	-414.234824	-1051.802434
1WMH.pdb (A-B)	-429.969989	-723.169349
1WMI.pdb (A-B)	-187.055211	-1013.508801
1WQJ.pdb (A-B)	-100.213873	-325.484753
1WWW.pdb (B-D)	-218.298688	-298.004388
1XG2.pdb (A-B)	-759.897654	-1028.255624
1YCP.pdb (D-E)	-136.643739	323.883651
1YCS.pdb (A-B)	-197.187166	-506.508176
1YDR.pdb (A-B)	-294.907279	-716.991589
1YPI.pdb (A-B)	-807.30125	-1366.42433
1YQV.pdb (B-C)	-352.974169	-539.047129
1Z7K.pdb (A-B)	-276.457116	-542.266286
2ARC.pdb (A-B)	-556.205635	-751.322595
2BF8.pdb (A-B)	-104.247264	-82.151554
2CCY.pdb (A-B)	-217.276789	-442.270179
2CTS.pdb (A-B)	-264.991195	-931.140895
2GN5.pdb (A-B)	0	0.44331

2HDH.pdb (A-B)	-730.516022	-1171.869902
2JEL.pdb (B-C)	-285.907811	-420.578471
2KAI.pdb (B-I)	-55.968261	-245.229261
2OHX.pdb (A-B)	-1226.794268	-1735.094258
2OR1.pdb (L-R)	-30.210904	-114.714654
2OZ9.pdb (A-B)	-345.773095	-782.369755
2PCC.pdb (A-B)	-456.953126	-568.827516
2PCH.pdb (A-B)	-1556.261954	-2395.175734
2PRG.pdb (B-C)	-124.159932	-308.871152
2PTC.pdb (A-B)	-412.268143	-675.613903
2RHE.pdb (A-B)	-426.754326	-575.360326
2RUS.pdb (A-B)	-817.287715	-1661.273255
2SIC.pdb (A-B)	-465.62034	-718.88683
2SNI.pdb (A-B)	-239.993022	-510.344012
2SOD.pdb (C-D)	-46.415505	-243.275765
2SPC.pdb (A-B)	-303.617417	-1247.839477
2TCT.pdb (A-B)	0	-531.23087
2TEC.pdb (A-B)	-316.384601	-566.725721
2THI.pdb (A-B)	0	-25.34322
2TMK.pdb (A-B)	-173.751082	-469.145692
2TNF.pdb (A-B)	-459.847923	-735.624553
2TRC.pdb (A-C)	-911.928854	-1737.150604
2TS1.pdb (A-B)	-72.595253	-400.438993
2TSC.pdb (A-B)	-844.971449	-1494.111809
3ENL.pdb (A-B)	-430.929972	-798.826972
3FAP.pdb (A-B)	-246.076069	-330.743839
3GRS.pdb (A-B)	-24.834058	-603.403948
3ICD.pdb (A-B)	-122.711993	-674.140023
3NOS.pdb (A-B)	-1270.944449	-2082.878779
3PVI.pdb (A-B)	-367.103287	-852.061737
3SDH.pdb (A-B)	-678.475905	-958.243425
3SDP.pdb (A-B)	-29.508741	-279.413761
3SGB.pdb (A-B)	-210.813983	-428.457953
3SSI.pdb (A-B)	0	-116.07727
3TPI.pdb (A-B)	-383.378496	-645.098086
4HTC.pdb (B-C)	-936.160607	-1484.771147
4MDH.pdb (A-B)	-790.227608	-1353.255288
5HVP.pdb (A-B)	-764.099305	-1353.996995
6GSV.pdb (A-B)	-966.536884	-1546.266054
6RLX.pdb (A-B)	-130.127427	309.570733

Supplementary Table ST8: The contribution of hydrogen bond energy and Van der Waals energy to the total energy for all entries in the 'without-water' dataset

PDB_ID (Interacting Chains)	Hydrogen Bond Energy	Van der Waals Energy
1A2K.pdb (A-B)	-42.906692	-558.049472
1A2K.pdb (A-D)	-61.566184	-301.751504
1A2K.pdb (C-A)	0	-7.99401
1A2Y.pdb (B-C)	-33.516576	-122.917196
1A2Z.pdb (A-B)	-45.873306	-497.093756
1A2Z.pdb (A-D)	-10.832955	-92.296155
1A3C.pdb (A-B)	-34.862977	-165.494297
1A4I.pdb (A-B)	-74.386892	-473.007692
1AA7.pdb (A-B)	-35.171254	-329.320524
1ACB.pdb (A-B)	-66.571445	-287.883365
1AFW.pdb (A-B)	-187.21928	-886.17586
1AK4.pdb (A-C)	0	0
1ALK.pdb (A-B)	-164.075265	-1444.958855
1AOR.pdb (A-B)	-77.589086	-508.265196
1ATL.pdb (A-B)	0	-72.97587
1AVW.pdb (A-B)	-55.235941	-416.262671
1AY7.pdb (A-B)	-47.063512	-318.886032
1B0N.pdb (A-B)	-39.54153	-598.25657
1B3A.pdb (A-B)	-81.894088	-350.538598
1B55.pdb (A-B)	-35.553247	-281.843437
1B66.pdb (A-B)	0	-6.8719
1B67.pdb (A-B)	-53.517542	-519.078612
1B93.pdb (A-B)	0	-24.61936
1B93.pdb (A-C)	-34.783476	-393.845406
1BAM.pdb (A-B)	0	-197.68285
1BCR.pdb (B-A)	-274.479092	-837.535992
1BFT.pdb (A-B)	-48.978995	-346.142805
1BIF.pdb (A-B)	-67.565202	-358.335442
1BJ1.pdb (C-D)	-77.17823	-514.61437
1BMQ.pdb (B-A)	-223.417756	-1041.953616
1BRS.pdb (A-D)	-53.185879	-408.660789
1BSR.pdb (A-B)	-93.14256	25.81307
1BTH.pdb (A-B)	-80.097611	340.486699
1BXG.pdb (A-B)	-69.861226	-375.096046
1C1Y.pdb (A-B)	-40.841529	-297.289549
1CDC.pdb (A-B)	-593.756929	-1796.654019
1CDT.pdb (A-B)	-26.864395	-146.955395
1CG2.pdb (A-B)	-18.972875	-74.368065
1CGI.pdb (A-B)	-67.622193	-396.195553
1CHO.pdb (C-D)	-50.28354	-205.39254
1COZ.pdb (A-B)	-74.74791	-372.36589
1CSE.pdb (A-B)	-78.063837	-332.932517
1CZJ.pdb (A-B)	-44.243303	-204.005223
1CZY.pdb (A-D)	-71.98455	-214.64872
1D2V.pdb (A-B)	-12.32925	-171.92501
1D2Z.pdb (A-B)	-46.883859	-289.246279
1DAN.pdb (B-C)	-35.509187	-137.387027
1DBF.pdb (A-B)	-41.237922	-135.320482
1DCP.pdb (A-B)	-47.238109	-245.599699
1DCP.pdb (A-C)	-39.372997	-148.277687
1DCP.pdb (A-D)	-6.185373	-96.812153
1DCP.pdb (A-E)	0	-37.49011

1DEL.pdb (A-B)	-26.487637	-230.850677
1DFJ.pdb (A-B)	-28.823078	-356.626878
1DFN.pdb (A-B)	-44.809082	-153.817082
1DHK.pdb (A-B)	-73.787808	-445.836508
1DKD.pdb (A-E)	-14.049294	-141.896984
1DQI.pdb (A-B)	-40.723294	-373.262944
1DQI.pdb (A-D)	-14.914089	-150.087509
1DS6.pdb (A-B)	-41.375393	-376.531083
1DVF.pdb (B-D)	-49.212778	-225.140388
1DVJ.pdb (A-B)	-12.07454	-58.4313
1DX5.pdb (I-M)	-52.620411	-309.497631
1DXG.pdb (A-B)	-130.280602	-402.295362
1E5D.pdb (A-B)	-62.04012	-524.53892
1E96.pdb (A-B)	-33.775908	-208.923438
1E98.pdb (A-B)	0	-140.18966
1EAY.pdb (A-C)	-23.874601	-183.240051
1EFN.pdb (A-B)	-17.226177	-264.475107
1EFU.pdb (A-B)	-97.289183	-658.739963
1EMV.pdb (A-B)	-30.332603	-333.127173
1EUV.pdb (A-B)	-144.56331	-768.38163
1EXT.pdb (A-B)	-40.63358	-323.14871
1F37.pdb (A-B)	-24.901908	-252.707298
1F74.pdb (A-C)	-30.557831	-537.845881
1F9Z.pdb (A-B)	-245.80708	-898.18312
1FDL.pdb (B-C)	-24.481942	-98.263502
1FIN.pdb (A-B)	-96.365953	-556.937693
1FIP.pdb (A-B)	-93.095152	-600.311142
1FLE.pdb (A-B)	-69.617172	-375.236362
1FM0.pdb (A-B)	-68.547918	-356.750758
1FNS.pdb (B-C)	-33.474425	-274.117095
1FS1.pdb (A-B)	0	-239.9005
1G6N.pdb (A-B)	0	-385.12391
1GG2.pdb (A-B)	-78.672949	-482.581109
1GL1.pdb (A-B)	0	-14.6778
1GLN.pdb (A-B)	-17.948343	-158.199403
1GOT.pdb (A-B)	-105.490201	-467.416601
1GUA.pdb (A-B)	-63.654245	-334.165185
1H2R.pdb (A-B)	-180.046845	-1301.257415
1HBN.pdb (B-C)	-242.98266	-1215.64803
1HBN.pdb (B-E)	-113.777098	-628.300178
1HFE.pdb (A-B)	-233.885784	-1423.317644
1HIA.pdb (B-I)	-73.007528	-327.062278
1HJR.pdb (A-C)	-17.009249	-272.126559
1HWG.pdb (A-B)	-32.849644	-444.633344
1I0H.pdb (A-B)	-26.582368	-303.402328
1ICW.pdb (A-B)	-91.566765	-388.026165
1IHF.pdb (B-A)	-129.48987	-842.47588
1J9L.pdb (A-B)	-18.889672	-79.670372
1JBU.pdb (A-C)	-71.976972	-440.159932
1JDH.pdb (A-B)	-131.873537	-712.251347
1JDP.pdb (A-H)	-11.120835	-205.048725
1JHG.pdb (A-B)	-34.117259	-627.288629
1JHL.pdb (B-C)	-14.474837	-171.934267
1JR8.pdb (A-B)	-21.425847	-386.594377
1JTH.pdb (A-B)	-27.224083	-370.498343
1K9O.pdb (A-B)	-61.639662	-361.556692
1KB5.pdb (B-H)	-15.128566	-85.473556

1KBA.pdb (A-B)	-43.761278	-184.472278
1KSH.pdb (A-B)	-93.126891	-350.379621
1KTZ.pdb (A-B)	-53.160177	-233.502227
1KVE.pdb (A-B)	-256.758548	-1112.395398
1KVE.pdb (A-C)	-3.24339	-81.33379
1L2I.pdb (A-C)	-16.825223	-147.468263
1LFD.pdb (A-B)	-65.414301	-293.802131
1LQV.pdb (B-D)	0	-86.8184
1LUC.pdb (A-B)	-69.255191	-730.154371
1LYA.pdb (A-B)	-440.278623	-1549.906473
1M4U.pdb (A-L)	-27.950988	-129.345988
1M9E.pdb (B-C)	-34.547469	-190.665469
1MCT.pdb (A-B)	-57.514525	-363.581305
1MEL.pdb (A-L)	-43.117137	-287.230847
1MJH.pdb (A-B)	-73.198588	-346.293848
1MKA.pdb (A-B)	-171.279862	-754.311622
1MLC.pdb (B-E)	-18.607764	-226.263104
1MSB.pdb (A-B)	-52.222091	-212.783011
1MZW.pdb (A-B)	-40.077778	-200.088488
1NCA.pdb (A-B)	-3.402811	-105.251021
1NF3.pdb (A-C)	-124.777382	-459.630922
1NL0.pdb (B-C)	-10.394474	-144.475204
1NMB.pdb (A-C)	-3.302939	-95.446979
1NW9.pdb (A-B)	-45.513636	-355.953636
1OC0.pdb (A-B)	-58.127641	-308.266861
1OEB.pdb (A-D)	-30.215621	-296.239871
1OEY.pdb (A-J)	-42.647712	-308.946782
1OPH.pdb (A-B)	-81.504961	-357.638971
1ORY.pdb (A-B)	-35.557761	-619.594621
1OSP.pdb (A-C)	0	-67.14015
1OTF.pdb (A-C)	-59.793689	-235.007439
1OTF.pdb (A-D)	-68.795105	-304.560795
1OTF.pdb (A-E)	-43.498236	-208.967566
1OTG.pdb (A-B)	-153.891051	-627.855051
1PGT.pdb (A-B)	-19.782544	-431.818594
1PHH.pdb (A-B)	0	-277.84866
1POI.pdb (B-A)	-104.442108	-645.077788
1POI.pdb (B-C)	-53.195986	-352.713156
1PP2.pdb (A-B)	-31.292664	-381.242234
1PPF.pdb (A-B)	-56.356729	-289.104789
1PYT.pdb (A-B)	-76.523947	-402.949707
1PYT.pdb (B-D)	-24.398453	-164.813453
1Q1S.pdb (B-C)	-107.059872	-417.947702
1QDL.pdb (B-A)	-47.113607	-428.896217
1QDN.pdb (A-B)	-8.739835	-164.435745
1QFX.pdb (A-B)	-155.474739	-1057.461859
1QH4.pdb (A-B)	-157.602012	-832.653352
1QKS.pdb (A-B)	-182.537846	-574.336586
1QSG.pdb (G-E)	-39.797982	-367.129592
1QSG.pdb (G-F)	-52.48432	-234.01531
1QSG.pdb (G-H)	-84.537116	-790.655406
1QTX.pdb (A-B)	-42.719787	-659.956127
1R0R.pdb (A-B)	-82.960704	-338.017004
1R3J.pdb (A-C)	-33.48249	-188.54715
1REG.pdb (A-B)	-63.550381	-304.695511
1REW.pdb (B-D)	-45.521732	-305.761992
1RP3.pdb (A-B)	-47.782273	-569.538303

1RPO.pdb (A-B)	0	-293.42267
1RYP.pdb (1-I)	-91.20847	-540.31109
1RYP.pdb (1-J)	-34.598169	-248.549269
1RYP.pdb (1-S)	-5.05743	-178.92359
1RYP.pdb (1-T)	-6.029211	-116.113281
1RYP.pdb (1-Z)	-38.197035	-253.402205
1RYP.pdb (1-2)	-52.565345	-304.206345
1S6C.pdb (A-B)	-51.489967	-198.919967
1SBB.pdb (A-B)	-11.898892	-139.924222
1SBW.pdb (A-I)	-77.781318	-333.194518
1SGP.pdb (A-B)	-75.577003	-273.943993
1SHW.pdb (A-B)	-9.151907	-160.044557
1SKO.pdb (A-B)	-166.988905	-581.267935
1SLW.pdb (A-B)	-63.756545	-287.202265
1SMT.pdb (A-B)	-23.719175	-622.898125
1SQ2.pdb (A-B)	-51.562996	-345.885036
1STF.pdb (A-B)	-43.972038	-281.119038
1SV0.pdb (B-D)	-47.927835	-269.661025
1SVF.pdb (B-A)	-27.520514	-297.798344
1SVF.pdb (C-D)	-11.192949	-246.713709
1T0F.pdb (A-C)	-67.682725	-511.306705
1T0J.pdb (B-C)	0	-218.02265
1TA3.pdb (A-B)	-19.773159	-269.611609
1TAB.pdb (A-B)	-47.144988	-252.285628
1TAW.pdb (A-B)	-63.200492	-343.762142
1TC1.pdb (A-B)	-73.075715	-545.787515
1TGS.pdb (A-B)	-84.218113	-383.735493
1TO2.pdb (A-B)	-78.735322	-388.768352
1TTW.pdb (A-B)	0	-112.084
1TVX.pdb (A-B)	-67.347872	-251.300332
1TVX.pdb (B-C)	0	-14.1361
1TX4.pdb (A-B)	-55.724998	-443.696388
1TY4.pdb (A-B)	0	7.204913
1U0S.pdb (A-Y)	-12.383116	-240.703866
1U6H.pdb (A-B)	-5.761313	-288.993093
1U8T.pdb (A-E)	-59.472345	-226.118025
1UAD.pdb (A-C)	-70.186224	-301.405804
1UJZ.pdb (A-B)	-63.450145	-381.672685
1US7.pdb (A-B)	-42.130683	-207.035363
1USU.pdb (A-B)	-66.696764	-356.190264
1UTG.pdb (A-B)	0	1609.85559
1VF6.pdb (A-C)	-49.232451	-379.191511
1VFB.pdb (B-C)	-30.287034	-121.639974
1VPP.pdb (A-C)	-85.060612	-377.582102
1WDC.pdb (A-B)	-66.798824	-636.665524
1WDC.pdb (A-C)	-54.390909	-691.958519
1WMH.pdb (A-B)	-56.449234	-349.648594
1WMI.pdb (A-B)	-187.055211	-1013.421801
1WQJ.pdb (A-B)	-37.398089	-262.665969
1WWW.pdb (B-D)	-22.292847	-101.998547
1XG2.pdb (A-B)	-44.827021	-313.184991
1YCP.pdb (D-E)	-45.619307	414.908083
1YCS.pdb (A-B)	-44.621741	-353.942751
1YDR.pdb (A-B)	-82.718274	-504.795584
1YPI.pdb (A-B)	-117.789068	-676.912148
1YQV.pdb (B-C)	-42.831414	-228.904374
1Z7K.pdb (A-B)	-72.363152	-338.172322

2ARC.pdb (A-B)	0	-195.11696
2BF8.pdb (A-B)	-35.325674	-12.606464
2CCY.pdb (A-B)	0	-224.99339
2CTS.pdb (A-B)	-264.991195	-931.140895
2GN5.pdb (A-B)	0	0.44331
2HDH.pdb (A-B)	-36.681394	-478.035274
2JEL.pdb (B-C)	-11.350914	-146.021574
2KAI.pdb (B-I)	-55.968261	-245.229261
2OHX.pdb (A-B)	-90.893186	-599.193176
2OR1.pdb (L-R)	-28.03247	-112.53622
2OZ9.pdb (A-B)	0	-436.59666
2PCC.pdb (A-B)	0	-111.85799
2PCH.pdb (A-B)	-168.993104	-1007.906884
2PRG.pdb (B-C)	-41.550097	-226.261317
2PTC.pdb (A-B)	-52.765907	-316.111667
2RHE.pdb (A-B)	-19.520738	-150.417688
2RUS.pdb (A-B)	-171.105421	-1015.090961
2SIC.pdb (A-B)	-83.770603	-337.037093
2SNI.pdb (A-B)	-71.766355	-342.093345
2SOD.pdb (C-D)	-46.415505	-242.210765
2SPC.pdb (A-B)	-67.926163	-1012.148223
2TCT.pdb (A-B)	0	-531.23087
2TEC.pdb (A-B)	-52.04928	-302.3824
2THI.pdb (A-B)	0	-25.34322
2TMK.pdb (A-B)	-15.236656	-310.630266
2TNF.pdb (A-B)	-47.718816	-323.415446
2TRC.pdb (A-C)	-167.665323	-992.878073
2TS1.pdb (A-B)	-72.595253	-400.438993
2TSC.pdb (A-B)	-57.301303	-706.440663
3ENL.pdb (A-B)	-38.874989	-435.349589
3FAP.pdb (A-B)	-3.645412	-88.312482
3GRS.pdb (A-B)	-24.834058	-603.403948
3ICD.pdb (A-B)	-122.711993	-674.140023
3IED.pdb (A-B)	-88.207786	-233.946316
3NOS.pdb (A-B)	-200.776286	-1012.710616
3PVI.pdb (A-B)	-70.349954	-555.308404
3SDH.pdb (A-B)	-36.260101	-316.027621
3SDP.pdb (A-B)	-10.77542	-260.68044
3SGB.pdb (A-B)	-68.229701	-285.873671
3SSI.pdb (A-B)	0	-116.07727
3TPI.pdb (A-B)	-57.843786	-319.563376
4CPA.pdb (A-I)	-16.289319	-181.209319
4HTC.pdb (B-C)	-104.942977	-653.323517
4MDH.pdb (A-B)	-97.057867	-660.085547
5HVP.pdb (A-B)	-185.859764	-774.112454
6GSV.pdb (A-B)	-29.128463	-608.857633
6RLX.pdb (A-B)	-66.652887	373.054273