Calculation of Van der Waals Energy:

V=4.184(VEi+Ej)[((Ri+Rj)/r)¹²-2((Ri+Rj)/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 q1 q2)/ 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/ron+1/rсн-1/roн-1/rcn) 332 * 4.184 kJ/mol

q₁= -0.42e & q₂=0.20e when H-hond forms between two amino acids. q₁= -0.42e & q₂=0.41e when H-hond forms between an amino acids and water and water acts as H-bond donor. q₁= -0.82e & q₂=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.



Without interface water...

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.



Non-Obligatory Complexes

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.



Obligatory Complexes

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- 2^{nd} bar). Relatively higher composition of hydrophobic residues in the protein as a whole (39 out of 77 cases; blue color- 3^{rd} 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	10RY.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	10SP.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	10TF.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	10TF.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	10TF.pdb A E 1.90	1T0F.pdb A C 1.85	2KAI.pdb B I 2.50
1A27. pdb A D 1.73	1DCP.pdb A D 2.30	110H. pdb A B 1.35	10TG.pdb A B 2,10	1T0J.pdb B C 2.00	20HX, pdb A B 1,80
1A3C, pdb A B 1,60	1DCP. pdb A E 2.30	1TCW.pdb A B 2.01	1PGT. pdb A B 1.80	1TA3.pdb A B 1.70	20R1.pdb L R 2.50
1A4T, pdb A B 1, 50	1DEL pdb A B 2.20	1THE pdb B A 2,50	1PHH, pdb A B 2, 30	ITAB, pdb A B 2, 30	2079. pdb A B 1.65
1AA7, pdb A B 2, 08	10E1.pdb A B 2.50	1191, pdb A B 1, 90	1POT ndb B A 2.50	ITAW, pdb A B 1,80	2PCC, pdb A B 2, 30
IACB pdb A B 2 00	IDEN pdb A B 1 90	1 IBU pdb A C 2 00	1POT pdb B C 2 50	1TC1 pdb A B 1 41	2PCH pdb A B 2 00
1AFW pdb A B 1 80	10HK pdb A B 1 85	11DH pdb A B 1 90	1PP2 ndb A B 2 50	ITGS pdb A B 1 80	2PRG pdb B C 2 30
14K4 pdb A D 2 36	10KD pdb A E 2 10	1 JDP odb A H 2 00	1PPE pdb A B 1 80	1T02 pdb A B 1 30	2PTC pdb A B 1 90
IALK pdb A B 2 AA	1001 pdb A B 1 70	11HG pdb A B 1 30	1PVT pdb A B 2 35	1TTW pdb A B 2 38	2RHE pdb A B 1 60
1AOR pdb A B 2 30	1001.pdb A D 1.70	1188 pdb A B 1 50	1PVT pdb B D 2 35	ITVX pdb A B 1 75	2RUS pdb A B 2 30
1ATL pdb A B 1 80	1056 pdb A B 2 35	1 TH pdb A B 2 00	1015 pdb B C 2 30	1TVX pdb B C 1 75	25TC pdb A B 1 80
1AW pdb A B 1 75	10VE pdb B D 1 90	1K90 pdb A B 2 30	1001 pdb B A 2 50	1TX4 pdb A B 1 65	2SNT pdb A B 2 10
1AV7 pdb A B 1 70	10V1 pdb A B 1 50	1KB5 pdb B H 2 50	100N pdb A B 2 30	1TV4 pdb A B 2 20	2500 pdb C D 2 00
1BON odb A B 1 90	10V5.pdb T M 2 30	1KBA pdb A B 2 30	10EX pdb A B 2 40	1105 pdb A V 1 90	2500.pdb C D 2.00
1834 pdb A B 1 60	10X5.pdb 1 H 2.50	1KSH pdb A B 1 80	10H4 pdb A B 1 41	116H pdb A B 2 38	2JCT pdb A B 2 10
1855 pdb A B 2 40	1550 pdb A B 2 50	1KTZ pdb A B 2 15	10KS pdb A B 1 29	100H. pdb A B 2.50	2TEC pdb A B 1 09
1866 pdb A B 1 00	1506 pdb A B 2.30	IKIZ. pdb A B 1 90	1056 pdb 6 E 1 75		2THT pdb A B 2 50
1967 pdb A B 1.90	1600 pdb A B 1 00	IKVE pdb A C 1 80	1056 pdb 6 E 1.75	10AD. pdb A C 2.10	2THL.pdb A B 2.50
1807. pdb A B 1.40	1ESC. pdb A C 2 00	11 2T odb A C 1.00	1056 pdb 6 H 1 75	1052.pdb A B 2.10	2THE pdb A B 1 40
1893. pdb A C 1 00	IEEN odb A B 2 50	ILED odb A R 2 10	10TV pdb A P 1 65	1057.pdb A B 2.50	2TRC pdb A C 2 40
184M pdb A B 1 95	1EFN. pdb A B 2.50	1LOV pdb R D 1 60	1808 pdb A B 1 10	1050.pdb A B 2.15	2TS1 pdb A B 2 30
1PCP pdb P A 2 50	1EMV pdb A B 1 70	1LC pdb A B 1 50	1821 pdb A C 1 99	1VE6 pdb A C 2 10	2151.pub A B 2.50
1PET odb A P 2 00	1EIN pdb A B 1.70	ILVA pdb A B 2 50	1855.pdb A C 1.90	IVEP pdb P C 1 90	215C.pdb A B 1.97
18FF. pdb A B 2.00	1EVV. pdb A B 1.00	1MAU pdb A L 2 42	IREG. pdb A B 1.90		SEND pdb A B 1 95
1811 pdb C D 2 40	1527 pdb A B 2 20	1040. pdb A L 2.42	1802 odb A B 2 20	IVPP. pdb A C 1.90	SFAP. PUD A B 1.05
1885 pdb 4 D 2 00	1F37. pdb A C 1 60	IMCT pdb A P 1 60	1800 pdb A B 1 40		SUNS. PUD A B 1.54
1PCP pdb A P 1 00	1607 pdb A C 1.00	IMEL pdb A L 2 50	18VD odb 1 T 1 00	IWMU odb A B 1 50	SICD. pdb A B 2.50
105K. pdb A B 1.90	1FTN pdb A B 2 20	IMIL pdb A P 1 70	187P. pdb 1 1 1.90	IWMT odb A B 2 20	SNUS. PUD A B 2.40
18VG pdb A B 2 30	1FID pdb A B 1 00	IMKA pdb A B 2 00	187P. pdb 1 5 1.90	1W01 pdb A B 1 60	SEVI. pdb A B 1.39
1C1V pdb A B 1 00	IFIF.pdb A B 1.90	IMIC pdb P E 2 50	187P. pdb 1 5 1.90	1WWW odb P D 2 20	3500 pdb A B 2 10
ICIT. pub A B 1.90	IFLE. PUD A B 1.90	IMCP odb A P 2 30	187P. pdb 1 7 1 00	1VG2 pdb A B 1 00	SSUP. PUD A B 2.10
ICDT odb A B 2.00	IFNG pdb B C 2 00	INSB. PUD A B 2.50	187P. pdb 1 2 1.90	IXO2. PUD A B 1.90	SSOB. PUD A B 1.00
1007. pdb A B 2.50	1FNS.pdb B C 2.00	INCA pdb A B 2.00	166C pdb A P 2 00	IVCS pdb A P 2 30	3551.pdb A B 2.50
1CGT pdb A B 2.30	ICEN pdb A B 2 10	INCA. pub A B 2.30	ISBR odb A B 2.00	IVOP odb A B 2.20	AUTC pdb B C 2 30
1CUO pdb C D 1 90	1662 pdb A B 2 40	INFS. pub A C 2.10	1500. pub A D 2.40	IVDT odb A B 1 00	AMOU odb A P 2 50
1007 pdb A B 2 00	1002. pub A B 2.40	INMP odb A C 2 20	1560 pdb A P 1 40	1VOV pdb P C 1 70	SHUD odb A P 2.00
1CCE pdb A B 1 20	LOLT DOL A B 2.10	10C0 pdb A R 2 20	150P. pub A B 1.40	177K pdb A P 1 00	SHVP. PUD A B 2.00
1CTL pdb A B 1.20	IGUI DOD A B 2.00	10C0.pdb A B 2.28	15HW. POD A B 2.20	12/K. pdb A B 1.90	COSV. pub A B 1.75
ICZY adb A B 2.10	100A.pdb A B 2.00	LUEB. POD A D 1.76	ISKU. pdb A B 2.00	ZARC. DOD A B 1.50	OKLX. POD A B 1.50
102V adb A D 2.00	INCK. DOD A B 1.40	LUEY. DOD A J 2.00	ISLW. POD A B 2.00	20F8. pdb A B 2.30	
102V.DOD A B 1.75	THEN. DOD B C 1.16	10PH. DOD A B 2.30	1502. DOD A B 1.45	2CCY. DOD A B 1.6/	

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	AB	2.50	1D2Z.pd	b A E	3 2.00	1HBN.pdb	BC	1.16	10EY.pdb	AJ	2.00	1SMT.pdb	AB	2.20	2CCY.pdb A B 1.6	57
1A2K.pdb	A D	2.50	1DAN.pd	b B C	2.00	1HBN.pdb	BE	1.16	10PH.pdb	AB	2.30	1502.pdb	AB	1.45	2CTS.pdb A B 2.0	0
1A2K.pdb	CA	2.50	1DBF.pd	b A E	3 1.30	1HFE.pdb	AB	1.60	10RY.pdb	AB	2.45	1STF.pdb	AB	2.37	2GN5.pdb A B 2.3	30
1A2Y.pdb	BC	1.50	1DCP.pd	b A E	3 2.30	1HIA.pdb	BI	2.40	10SP.pdb	AC	1.95	1SV0.pdb	B D	2.07	2HDH.pdb A B 2.2	20
1A2Z.pdb	AB	1.73	1DCP.pd	b A C	2.30	1HJR.pdb	AC	2.50	10TF.pdb	AC	1.90	1SVF.pdb	BA	1.40	2JEL.pdb B C 2.5	0
1A2Z.pdb	A D	1.73	1DCP.pd	b A D	2.30	1HWG.pdb	AB	2.50	10TF.pdb	A D	1.90	1SVF.pdb	C D	1.40	2KAI.pdb B I 2.5	0
1A3C. pdb	AB	1.60	1DCP.pd	b A F	2.30	1TOH. pdb	AB	1.35	10TF. pdb	AE	1.90	1TOF. pdb	AC	1.85	20HX.pdb A B 1.8	30
1A4I.pdb	AB	1.50	1DEL.pd	b A E	3 2.20	1ICW.pdb	AB	2.01	10TG.pdb	AB	2.10	1T0J.pdb	BC	2.00	20R1.pdb L R 2.5	0
1AA7. pdb	AB	2.08	1DFJ.pd	b A E	3 2.50	1THF.pdb	BA	2.50	1PGT.pdb	AB	1.80	1TA3.pdb	AB	1.70	2079.pdb A B 1.6	55
1ACB. pdb	AB	2.00	1DFN.pd	b A E	3 1.90	1.19L. pdb	AB	1.90	1PHH, pdb	AB	2.30	1TAB. pdb	AB	2.30	2PCC.pdb A B 2.3	30
1AFW.pdb	AB	1.80	1DHK.pd	b A E	3 1.85	1JBU. pdb	AC	2.00	1POT. pdb	BA	2.50	1TAW. pdb	AB	1.80	2PCH. pdb A B 2.0	00
1AK4. pdb	A D	2.36	1DKD.pd	b A E	2.10	1JDH. pdb	AB	1.90	1POT. pdb	BC	2.50	1TC1.pdb	AB	1.41	2PRG. pdb B C 2.3	30
1ALK. pdb	AB	2.00	1DOT.pd	b A E	3 1.70	1JDP. pdb	AH	2.00	1PP2. pdb	AB	2.50	1TGS. pdb	AB	1.80	2PTC. pdb A B 1.9	0
1AOR. pdb	AB	2.30	1DOI.pd	b A D	1.70	1JHG.pdb	AB	1.30	1PPF.pdb	AB	1.80	1T02.pdb	AB	1.30	2RHE.pdb A B 1.6	50
1ATL.pdb	AB	1.80	1DS6.pd	b A E	3 2.35	1JHL.pdb	BC	2.40	1PYT.pdb	AB	2.35	1TTW.pdb	AB	2.38	2RUS.pdb A B 2.3	30
1AVW.pdb	AB	1.75	1DVF.pd	b B D	1.90	1JR8. pdb	AB	1.50	1PYT.pdb	BD	2.35	1TVX.pdb	AB	1.75	2SIC.pdb A B 1.8	30
1AY7. pdb	AB	1.70	1DVJ.pd	b A E	3 1.50	1JTH. pdb	AB	2.00	1015.pdb	BC	2.30	1TVX.pdb	BC	1.75	2SNI. pdb A B 2.1	0
1BON, pdb	AB	1.90	1DX5.pd	b T M	1 2.30	1K90.pdb	AB	2.30	10DL pdb	BA	2.50	1TX4.pdb	AB	1.65	250D.pdb C D 2.0	00
1B3A.pdb	AB	1.60	1DXG.pd	b A F	3 1.80	1KB5. pdb	BH	2.50	10DN, pdb	AB	2.30	1TY4. pdb	AB	2.20	2SPC. pdb A B 1.8	30
1855.pdb	AB	2.40	1E5D.pd	b A E	3 2.50	1KBA.pdb	AB	2.30	10FX.pdb	AB	2.40	1UOS.pdb	AY	1.90	2TCT.pdb A B 2.1	0
1866.pdb	AB	1.90	1E96.pd	b A E	3 2.40	1KSH. pdb	AB	1.80	10H4.pdb	AB	1.41	1U6H.pdb	AB	2.38	2TEC.pdb A B 1.9	8
1867.pdb	AB	1.48	1E98.pd	b A E	3 1.90	1KTZ.pdb	AB	2.15	10KS.pdb	AB	1.28	1U8T.pdb	AE	1.50	2THI. pdb A B 2.5	0
1893. pdb	AB	1.90	1EAY.pd	b A C	2.00	1KVE.pdb	AB	1.80	10SG.pdb	GE	1.75	1UAD, pdb	AC	2.10	2TMK. pdb A B 2.4	10
1893. pdb	AC	1.90	1EEN. pd	b A E	3 2.50	1KVE.pdb	AC	1.80	10SG. pdb	GE	1.75	1UJZ.pdb	AB	2.10	2TNF. pdb A B 1.4	10
1BAM, pdb	AB	1.95	1EFU.pd	b A E	3 2.50	1L2I.pdb	AC	1.95	10SG.pdb	GH	1.75	1US7.pdb	AB	2.30	2TRC.pdb A C 2.4	10
1BCR.pdb	BA	2.50	1EMV.pd	b A E	3 1.70	1LFD.pdb	AB	2.10	10TX.pdb	AB	1.65	1USU.pdb	AB	2.15	2TS1.pdb A B 2.3	30
1BFT.pdb	AB	2.00	1EUV.pd	b A E	3 1.60	1LOV.pdb	BD	1.60	1ROR. pdb	AB	1.10	1UTG.pdb	AB	1.34	2TSC.pdb A B 1.9	7
1BIF.pdb	AB	2.00	1EXT.pd	b A E	3 1.85	1LUC.pdb	AB	1.50	1R3J.pdb	AC	1.90	1VF6.pdb	AC	2.10	3ENL.pdb A B 2.2	25
1BJ1.pdb	CD	2.40	1F37.pd	b A E	3 2.30	1LYA.pdb	AB	2.50	1REG.pdb	AB	1.90	1VFB.pdb	BC	1.80	3FAP.pdb A B 1.8	35
1BMO.pdb	BA	2.50	1F74.pd	b A C	1.60	1M4U.pdb	AL	2.42	1REW.pdb	BD	1.86	1VPP.pdb	AC	1.90	3GRS.pdb A B 1.5	14
1BRS.pdb	A D	2.00	1F9Z.pd	b A E	3 1.50	1M9E.pdb	BC	1.72	1RP3.pdb	AB	2.30	1WDC.pdb	AB	2.00	3ICD.pdb A B 2.5	0
1BSR.pdb	AB	1.90	1FDL.pd	b B C	2.50	1MCT.pdb	AB	1.60	1RPO.pdb	AB	1.40	1WDC.pdb	AC	2.00	3IED.pdb A B 2.0	1
1BTH.pdb	AB	2.30	1FIN.pd	b A E	3 2.30	1MEL.pdb	AL	2.50	1RYP.pdb	1 I	1.90	1WMH.pdb	AB	1.50	3NOS.pdb A B 2.4	0
1BXG.pdb	AB	2.30	1FIP.pd	b A E	3 1.90	1MJH.pdb	AB	1.70	1RYP.pdb	1 J	1.90	1WMI.pdb	AB	2.30	3PVI.pdb A B 1.5	9
1C1Y.pdb	AB	1.90	1FLE.pd	b A E	3 1.90	1MKA.pdb	AB	2.00	1RYP.pdb	1 S	1.90	1WQJ.pdb	AB	1.60	3SDH.pdb A B 1.4	10
1CDC.pdb	AB	2.00	1FM0.pd	b A E	3 1.45	1MLC.pdb	BE	2.50	1RYP.pdb	1 T	1.90	1WWW.pdb	B D	2.20	3SDP.pdb A B 2.1	0
1CDT.pdb	AB	2.50	1FNS.pd	b B C	2.00	1MSB.pdb	AB	2.30	1RYP.pdb	1 Z	1.90	1XG2.pdb	AB	1.90	3SGB.pdb A B 1.8	30
1CG2.pdb	AB	2.50	1FS1.pd	b A E	3 1.80	1MZW.pdb	AB	2.00	1RYP.pdb	12	1.90	1YCP.pdb	DE	2.50	3SSI.pdb A B 2.3	30
1CGI.pdb	AB	2.30	1G6N.pd	b A E	3 2.10	1NCA.pdb	AB	2.50	1S6C.pdb	AB	2.00	1YCS.pdb	AB	2.20	3TPI.pdb A B 1.9	0
1CHO.pdb	CD	1.80	1GG2.pd	b A E	3 2.40	1NF3.pdb	AC	2.10	1SBB.pdb	AB	2.40	1YDR.pdb	AB	2.20	4CPA.pdb A I 2.5	Ø
1COZ.pdb	AB	2.00	1GL1.pd	b A E	3 2.10	INLO.pdb	BC	2.20	1SBW.pdb	AI	1.80	1YPI.pdb	AB	1.90	4HTC.pdb B C 2.3	30
1CSE.pdb	AB	1.20	1GLN.pd	AE	3 2.50	1NMB.pdb	AC	2.20	1SGP.pdb	AB	1.40	1YQV.pdb	BC	1.70	4MDH.pdb A B 2.5	O
1CZJ.pdb	AB	2.16	1GOT.pd	b A E	3 2.00	1NW9.pdb	AB	2.40	1SHW.pdb	AB	2.20	1Z7K.pdb	AB	1.90	5HVP.pdb A B 2.0	00
1CZY.pdb	A D	2.00	1GUA.pd	AE	3 2.00	10C0.pdb	AB	2.28	1SKO.pdb	AB	2.00	2ARC.pdb	AB	1.50	6GSV.pdb A B 1.7	15
1D2V.pdb	AB	1.75	1H2R.pd	b A E	3 1.40	10EB.pdb	A D	1.76	1SLW.pdb	AB	2.00	2BF8.pdb	AB	2.30	6RLX.pdb A B 1.5	0

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 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 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 NHAc 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 NHAc 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
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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 A796 CB215 ASP B3613 CB8.30698.21489184 LYS A1453 CB184 LYS B3369 CB9.20631.99242215 ASP A1697 CB101 ASP B2712 CB7.89729.06523

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 -0.017617881 ARG A 1306 C 86 ILE B 5453 HD11 5.94845 -0.0054672481 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 -0.0029262281 ARG A 1306 C 110 LEU B 5811 CD2 6.5056 -0.020253881 ARG A 1306 C 110 LEU B 5817 HD11 6.57597 -0.0030043881 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 -0.0024414181 ARG A 1307 O 86 ILE B 5444 CD1 6.27556 -0.018698881 ARG A 1307 O 86 ILE B 5453 HD11 5.42406 -0.006381281 ARG A 1307 86 ILE B 5454 HD12 6.37311 0 -0.00243434 81 ARG A 1307 86 ILE B 5455 HD13 6.29708 -0.00261566 0 81 ARG A 1307 O 110 LEU B 5809 CG 6.73687 -0.0122485O 110 LEU B 5810 CD1 6.6822 81 ARG A 1307 -0.012859

81 ARG A 1307 0 110 LEU B 5811 CD2 5.6518 -0.0348194 81 ARG A 1307 0 110 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.

1A2K, pdb -357, 849239 -873, 607019 1A2K, pdb (A-D) -364, 696362 -544, 917682 1A2K, pdb (B-C) -368, 601714 -458, 002334 1A2Z, pdb (A-D) -44, 430637 -128, 893837 1A3C, pdb (A-B) -363, 610532 -1236, 231332 1AA7, pdb (A-B) -234, 936985 -589, 086255 1ACB, pdb (A-B) -144, 810703 -367, 157623 1AK4, pdb (A-B) -1748, 075349 -2447, 032929 1AK4, pdb (A-B) -164, 075265 -1444, 958855 1ACB, pdb (A-B) -435, 309143 -925, 985253 1ATL, pdb (A-B) -435, 503777 -418, 529647 1AVW, pdb (A-B) -144, 787613 -716, 610133 1BON, pdb (A-B) -435, 503777 -418, 529647 1AVW, pdb (A-B) -23, 37649 -30, 2552 1AS, pdb (A-B) -23, 37649 -30, 2552 1B67, pdb (A-B) -23, 37649 -30, 2552 1B67, pdb (A-B) -26, 16209 -98, 3362 <	PDB_ID (I	Interacting Chains)	Hydrogen-Bond Energy	Van der Waals Energy
1A2K, pdb -304.696362 -544.917682 1A2Y, pdb (C-A) 0 -7.99401 1A2Y, pdb (A-B) -559.540616 -109.247066 1A22, pdb (A-B) -44.430637 -125.893837 1A3C, pdb (A-B) -837.610532 -1236.231332 1AA7, pdb (A-B) -294.936965 -559.066255 1ACE, pdb (A-B) -145.818703 -37.157623 1AFW, pdb (A-B) -144.80637 -1444.958855 1AOR, pdb (A-B) -1478.075265 -1444.958855 1AOR, pdb (A-B) -169.075265 -1444.958855 1AOR, pdb (A-B) -149.693283 -550.720013 1AY7, pdb (A-B) -149.693283 -550.720013 1AY7, pdb (A-B) -324.775401 -88.526441 1B3A, pdb (A-B) -247.303166 -662.220356 1B66, pdb (A-B) -247.389354 -606.451284 1B3A, pdb (A-B) -273.37649 -30.25522 1B67, pdb (A-B) -28.834002 -551.36312 1B33, pdb (A-B)	1A2K.pdb	(A-B)	-357.849239	-873.607019
1A2R.pdb (B=C) -368.601714 -458.002334 1A2Z.pdb (A=B) -559.540616 -1009.247066 1A3C.pdb (A=B) -44.430637 -125.893837 1A3C.pdb (A=B) -34.862977 -165.494297 1A41.pdb (A=B) -234.936985 -559.686255 1ACB.pdb (A=B) -145.818703 -367.157623 1AT.pdb (A=B) -144.075265 -144.958855 1ACB.pdb (A=B) -164.075265 -144.958855 1AOR.pdb (A=B) -444.787613 -265.985253 1ATL.pdb (A=B) -444.787613 -716.10133 1AY7.pdb (A=B) -144.958855 -268.04241 1AY7.pdb (A=B) -144.787613 -716.10133 1BN.pdb (A=B) -129.963283 -550.720013 1AY7.pdb (A=B) -224.775401 -883.526441 1B3A.pdb (A=B) -679.960383 -948.604893 1B55.pdb (A=B) -23.37649 -30.25522 1B67.pdb (A=B) -24.834002 -53.453362 1B33.pdb (A=B) -24.834002 -53.453362 1B49.pdb (A=B) -24.834002 -53.453362 1B55.pdb (A=B) -24.834002 -53.453362	1A2K.pdb	(A-D)	-304.696362	-544.917682
1A2r.pdb (A=C) -368.601714 -458.002334 1A2r.pdb (A=D) -44.430637 -1059.247066 1A2r.pdb (A=B) -34.862977 -165.494297 1A4r.pdb (A=B) -234.862977 -165.494297 1A4r.pdb (A=B) -244.936985 -589.086255 1ACB.pdb (A=B) -145.818703 -67.157623 1Arw.pdb (A=B) -145.818703 -624.7032929 1AK.pdb (A=C) 0 0 1ALK.pdb (A=B) -145.05327 -144.958855 1AOR.pdb (A=B) -495.309143 -925.985253 1AT.pdb (A=B) -495.309143 -925.985253 1AW.pdb (A=B) -444.787613 -716.610133 1BN.pdb (A=B) -644.775401 -883.526441 1BAA.pdb (A=B) -619.960383 -948.604893 1BS5.pdb (A=B) -23.37649 -30.25522 1B67.pdb (A=B) -224.775401 -883.526441 1BAA.pdb (A=B) -23.37649 -30.25522 1B67.pdb (A=B) <t< td=""><td>1A2K.pdb</td><td>(C-A)</td><td>0</td><td>-7.99401</td></t<>	1A2K.pdb	(C-A)	0	-7.99401
1A2z.pdb (A-D) -559.540616 -1009.247066 1A2z.pdb (A-D) -44.430637 -125.893837 1A3c.pdb (A-B) -34.662977 -165.494297 1A41.pdb (A-B) -294.936985 -589.086255 1ACB.pdb (A-B) -145.818703 -367.157623 1AK4.pdb (A-B) -1448.076349 -2447.032929 1AK4.pdb (A-C) 0 0 1AK4.pdb (A-B) -164.075265 -1444.958855 1ACB.pdb (A-B) -495.309143 -925.985253 1ATL.pdb (A-B) -495.309143 -925.985253 1ATL.pdb (A-B) -189.693283 -550.720013 1AY7.pdb (A-B) -244.775401 -883.526441 1BSA.pdb (A-B) -244.737613 -716.610133 1BS5.pdb (A-B) -247.389354 -662.20356 1B66.pdb (A-B) -248.34002 -53.45362 1B3.pdb (A-B) -247.389354 -666.451284 1B3.pdb (A-B) -268.34002 -53.43362 1B3.pdb (A-B)	1A2Y.pdb	(B-C)	-368.601714	-458.002334
1A2C.pdb (A-D) -44.430637 -125.693837 1A3C.pdb (A-B) -34.862977 -165.494297 1A41.pdb (A-B) -837.610532 -1236.231332 1AA7.pdb (A-B) -249.936985 -589.086255 1ACR.pdb (A-B) -145.818703 -367.157623 1AFW.pdb (A-B) -1748.076349 -2447.032929 1AK.kpdb (A-C) 0 0 1ALK.pdb (A-B) -164.075265 -1444.958855 1AOR.pdb (A-B) -495.309143 -925.985253 1ATL.pdb (A-B) -445.513777 -418.529647 1AW.pdb (A-B) -1499.693283 -550.720013 1AY.pdb (A-B) -324.775401 -883.526441 1BSA.pdb (A-B) -679.960383 -948.604893 1B55.pdb (A-B) -662.20356 1682.202152 1B67.pdb (A-B) -247.389354 -664.252842 1B33.pdb (A-B) -28.834002 -53.453362 1B93.pdb (A-B) -249.883013 -117.68285 1B68.pdb (A-B) <td>1A2Z.pdb</td> <td>(A-B)</td> <td>-559.540616</td> <td>-1009.247066</td>	1A2Z.pdb	(A-B)	-559.540616	-1009.247066
1A3C.pdb -34.862977 -165.494297 1A4T.pdb (A=B) -837.610532 -1236.231332 1AA7.pdb (A=B) -244.936985 -589.086255 1ACB.pdb (A=B) -145.818703 -367.157623 1AFW.pdb (A-C) 0 0 1ALK.pdb (A-C) 0 0 1ALK.pdb (A-B) -164.075265 -1444.958855 1AN7.pdb (A-B) -495.309143 -925.985253 1ATL.pdb (A-B) -345.553777 -418.529647 1AW.pdb (A-B) -149.693283 -550.720013 1AW.pdb (A-B) -1444.958055 -885.526441 1B3A.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -28.834002 -53.453362 1B33.pdb (A-B) -2447.389354 -606.451284 1B39.pdb (A-B) -247.389354 -606.451284 1B39.pdb (A-B) -279.688013 -717.124153 1B7.pdb (A-B) -265.16209 -368.3344	1A2Z.pdb	(A-D)	-44.430637	-125.893837
1A47.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-B) -164.075265 -1444.958855 1ADR.pdb (A-B) -495.309143 -925.985253 1ATL.pdb (A-B) -485.553777 -418.529647 1AW.pdb (A-B) -189.693283 -550.720013 1AY7.pdb (A-B) -444.787613 -716.610133 1BON.pdb (A-B) -679.960383 -946.604893 1BS5.pdb (A-B) -679.960383 -946.604893 1BS5.pdb (A-B) -679.960383 -946.604893 1BS5.pdb (A-B) -223.7649 -30.2522 1B67.pdb (A-B) -284.834002 -53.453662 1B93.pdb (A-B) -248.34002 -53.45362 1BS7.pdb (A-B) -2498.349104 -2061.407004 1BS7.pdb (A-B) -64.198907 -361.362717 1BFT.pdb	1A3C.pdb	(A-B)	-34.862977	-165.494297
$\begin{array}{llllllllllllllllllllllllllllllllllll$	1A4I.pdb	(A-B)	-837.610532	-1236.231332
1ACB.pdb -145.818703 -367.157623 1AFW.pdb (A-B) -1748.076349 -2447.032929 1AK4.pdb (A-B) -164.075265 -1444.958855 1AOR.pdb (A-B) -345.553777 -418.529647 1ATL.pdb (A-B) -345.553777 -418.529647 1AWV.pdb (A-B) -345.753777 -418.529647 1AWV.pdb (A-B) -342.775401 -883.5526441 1B3A.pdb (A-B) -324.775401 -883.5526441 1B3A.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -28.834002 -53.453362 1B93.pdb (A-B) -247.389354 -606.451284 1B3A.pdb (A-B) -247.389354 -606.451284 1B3A.pdb (A-B) -248.34002 -53.453362 1B93.pdb (A-B) -247.389354 -606.451284 1B3A.pdb (A-B) -247.389354 -606.451284 1B3A.pdb (A-B) -247.389354 -606.4513284 1B3A.pdb (A-B)	1AA7.pdb	(A-B)	-294.936985	-589.086255
$\begin{array}{llllllllllllllllllllllllllllllllllll$	1ACB.pdb	(A-B)	-145.818703	-367.157623
$\begin{array}{llllllllllllllllllllllllllllllllllll$	1AFW.pdb	(A-B)	-1748.076349	-2447.032929
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 1BON.pdb (A-B) -324.775401 -883.526441 1B3A.pdb (A-B) -679.960383 -948.604893 1B55.pdb (A-B) -213.37649 -30.25522 1B66.pdb (A-B) -28.834002 -53.453362 1B67.pdb (A-B) -247.389354 -660.451284 1B3A.pdb (A-B) -247.389354 -660.451284 1BAM.pdb (A-B) -1498.349104 -2061.407004 1BFT.pdb (A-B) -67.565202 -358.335442 1BJ1.pdb (C-D) -279.688013 -717.124153 1BSR.pdb (A-B) -625.16209 -980.637 1BSR.pdb (A-B) -363.305094 -668.539914 ICCT.pdb (A-B) -250.227808 169.819502 1BKR.pdb	1AK4.pdb	(A-C)	0	0
1AOR.pdb (A-B) -495.309143 -925.985253 1ATW.pdb (A-B) -345.553777 -418.529647 1AWW.pdb (A-B) -169.693283 -550.720013 1AY7.pdb (A-B) -444.787613 -716.610133 1BNN.pdb (A-B) -324.775401 -883.526441 1B3A.pdb (A-B) -679.960383 -948.604893 1B55.pdb (A-B) -218.930166 -662.220356 1B66.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -28.834002 -53.453362 1B93.pdb (A-C) -247.389354 -606.451284 1B93.pdb (A-C) -247.389354 -606.451284 1BMM.pdb (A-B) 0 -197.68285 1BER.pdb (B-A) -1498.349104 -2061.407004 1BFT.pdb (A-B) -67.565202 -358.335442 1BJI.pdb (A-B) -67.565202 -358.335442 1BSR.pdb (A-B) -791.959222 -673.003592 1BTT.pdb (A-B) -250.227808 169.819502 1BSG.pdb (A-	1ALK.pdb	(A-B)	-164.075265	-1444.958855
1ATL.pdb (A-B) -345.553777 -418.529647 1AWT.pdb (A-B) -189.693283 -550.720013 1AYT.pdb (A-B) -444.787613 -716.610133 1BON.pdb (A-B) -324.775401 -883.526441 1B3A.pdb (A-B) -679.960383 -948.604893 1B55.pdb (A-B) -215.930166 -662.220356 1B66.pdb (A-B) -23.37649 -30.25522 1B67.pdb (A-B) -28.834002 -53.453362 1B93.pdb (A-B) -28.834002 -53.453362 1B93.pdb (A-B) -1498.349104 -2061.407004 1B91.pdb (A-B) -64.198907 -361.362717 1BFT.pdb (A-B) -67.565202 -358.335442 1BJ1.pdb (A-B) -625.16209 -980.637 1BSR.pdb (A-D) -625.16209 -980.637 1BSR.pdb (A-B) -719.959222 -673.003592 1BTH.pdb (A-B) -361.532653 -617.980673 1C1Y.pdb (A-B) -361.532653 -617.980673 1C2C.pdb (1AOR.pdb	(A-B)	-495.309143	-925.985253
1AVW.pdb(A-B)-189.693283-550.7200131AY7.pdb(A-B)-444.787613-716.6101331B0N.pdb(A-B)-324.775401-883.5264411B3A.pdb(A-B)-679.960383-948.6048931B55.pdb(A-B)-415.930166-662.2203561B66.pdb(A-B)-23.37649-30.255221B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-67.565202-358.3354221BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CGI.pdb(A-B)-95.441015-424.0143751CGI.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0143751CCZ.pdb(A-B)-95.441015-424.0	1ATL.pdb	(A-B)	-345.553777	-418.529647
1AY7.pdb(A-B)-444.787613-716.6101331B0N.pdb(A-B)-324.775401-883.5264411B3A.pdb(A-B)-679.960383-948.6048931B55.pdb(A-B)-415.930166-662.2203561B66.pdb(A-B)-23.37649-30.255221B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-B)-247.389354-606.4512841B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-64.198907-361.3627171BIF.pdb(A-B)-652.16202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-361.305094-668.5399141CUT.pdb(A-B)-361.305094-668.5399141CUT.pdb(A-B)-361.52653-617.9806731CDC.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424	1AVW.pdb	(A-B)	-189.693283	-550.720013
1B0N.pdb-324.775401-883.5264411B3A.pdb(A-B)-679.960383-948.6048931B55.pdb(A-B)-415.930166-662.2203561B66.pdb(A-B)-23.37649-30.255221B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-C)-247.389354-606.4512841B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BTF.pdb(A-B)-67.565202-358.3354221BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-361.32653-617.9806731CDC.pdb(A-B)-361.32653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.44303-204.0052231CZ1.pdb(A-B)-48.693309-703.5619891C22.pdb(A-B)-48.66655-649.2224151D2V.pdb(A-B)-48.626655-649.2224151D2V.pdb(A-B)-48.626655-649.2224151D2V.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.962528	1AY7.pdb	(A-B)	-444.787613	-716.610133
1B3A.pdb-679.960383-948.6048931B55.pdb(A-B)-415.930166-662.2203561B66.pdb(A-B)-23.37649-30.255221B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-B)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BFT.pdb(A-B)-64.198907-361.3627171BFT.pdb(A-B)-67.565202-358.3354421BJ1.pdb(A-B)-67.565202-358.3354421BJ1.pdb(A-B)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BSR.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-95.441015-424.0143751CGI.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-290.002746-589.7877261CS2.pdb(A-B)-448.693309-703.5618991CZJ.pdb(A-B)-449.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-489.626655-649.222415	1B0N.pdb	(A-B)	-324.775401	-883.526441
1B55.pdb(A-B)-415.930166-662.2203561B66.pdb(A-B)-23.37649-30.255221B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-B)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-64.198907-361.3627171BIF.pdb(A-B)-67.565202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-57.505316-177.5963161CGI.pdb(A-B)-95.441015-424.0143751CGI.pdb(A-B)-95.441015-424.0143751CGI.pdb(A-B)-95.441015-424.0143751CC2.pdb(A-B)-95.441015-424.0143751CC2.pdb(A-B)-95.441015-424.0143751CC2.pdb(A-B)-95.441015-424.0143751CC2.pdb(A-B)-95.6557-459.6708271D2V.pdb(A-B)-448.69303-703.5619891C2J.pdb(A-B)-448.69303-204.0052231C2J.pdb(A-B)-448.69303-204.0052231D2V.pdb(A-B)-448.626655-649.2224151D2V.pdb(A-B)-468.688-292.962528 <td>1B3A.pdb</td> <td>(A-B)</td> <td>-679.960383</td> <td>-948.604893</td>	1B3A.pdb	(A-B)	-679.960383	-948.604893
1B66.pdb -23.37649 -30.25522 1B67.pdb (A-B) -186.806242 -652.369312 1B93.pdb (A-C) -247.389354 -606.451284 1B93.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-B) -791.959222 -673.003592 1BTH.pdb (A-B) -250.227808 169.819502 1BXG.pdb (A-B) -361.532653 -617.980673 1CDC.pdb (A-B) -361.532653 -617.980673 1CDC.pdb (A-B) -1277.646318 -2480.783408 1CDT.pdb (A-B) -80.239687 -135.634877 1CGI.pdb (A-B) -95.441015 -424.014375 1CMO.pdb (C-D) -151.052859 -306.161859 1CG2.pdb (A-B) -290.002746 -589.787726 1CSE.pdb (A-B) -	1B55.pdb	(A-B)	-415.930166	-662.220356
1B67.pdb(A-B)-186.806242-652.3693121B93.pdb(A-B)-28.834002-53.4533621B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-64.198907-361.3627171BIF.pdb(A-B)-67.565202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-95.441015-424.0143751CG1.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG2.pdb(A-B)-90.002746-589.7877261CS2.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-410.482313-708.1648731DDP.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-614.082313-708.164873	1B66.pdb	(A-B)	-23.37649	-30.25522
1B93.pdb-28.834002-53.4533621B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-64.198907-361.3627171BIF.pdb(A-B)-67.565202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BSR.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-55.441015-424.0143751CG2.pdb(A-B)-95.441015-424.0143751CG1.pdb(A-B)-290.002746-589.7877261CS2.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.693303-204.0052231CZY.pdb(A-B)-448.62655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-110.084688-292.9625281DBF.pdb(A-B)-411.64873-708.1648731DCP.pdb(A-B)-614.082313-708.164873	1B67.pdb	(A-B)	-186.806242	-652.369312
1B93.pdb(A-C)-247.389354-606.4512841BAM.pdb(A-B)0-197.682851BCR.pdb(B-A)-1498.349104-2061.4070041BFT.pdb(A-B)-64.198907-361.3627171BIF.pdb(A-B)-67.565202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-B)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591CO2.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.693303-204.0052231CZY.pdb(A-B)-448.62655-649.2224151D2V.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-614.082313-708.164873	1B93.pdb	(A-B)	-28.834002	-53.453362
IBAM.pdb0-197.68285IBCR.pdb(B-A)-1498.349104-2061.407004IBFT.pdb(A-B)-64.198907-361.362717IBIF.pdb(A-B)-67.565202-358.335442IBJ1.pdb(C-D)-279.68013-717.124153IBRS.pdb(A-D)-625.16209-980.637IBSR.pdb(A-B)-791.959222-673.003592IBTH.pdb(A-B)-250.227808169.819502IBXG.pdb(A-B)-361.532653-617.980673ICDC.pdb(A-B)-361.532653-617.980673ICDC.pdb(A-B)-57.505316-177.596316ICG2.pdb(A-B)-95.441015-424.014375ICG1.pdb(A-B)-95.441015-424.014375ICC2.pdb(A-B)-290.002746-589.787726ICS2.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693303-224.005223IDZZ.pdb(A-B)-448.693303-224.005223IDZZ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.692313-708.164873IDZZ.pdb(A-B)-448.692313-708.164873 </td <td>1B93.pdb</td> <td>(A-C)</td> <td>-247.389354</td> <td>-606.451284</td>	1B93.pdb	(A-C)	-247.389354	-606.451284
IBCR.pdb-1498.349104-2061.407004IBFT.pdb(A-B)-64.198907-361.362717IBIF.pdb(A-B)-67.565202-358.335442IBJ1.pdb(C-D)-279.688013-717.124153IBRS.pdb(A-D)-625.16209-980.637IBSR.pdb(A-B)-791.959222-673.003592IBTH.pdb(A-B)-250.227808169.819502IBXG.pdb(A-B)-361.532653-617.980673ICC.pdb(A-B)-361.532653-617.980673ICDC.pdb(A-B)-57.505316-177.596316ICG2.pdb(A-B)-95.441015-424.014375ICG2.pdb(A-B)-95.441015-424.014375ICO2.pdb(A-B)-290.002746-589.787726ICSE.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.67657-459.670827IDZ2.pdb(A-B)-49.02655-649.222415IDZ2.pdb(A-B)-411.414308-653.800728IDAN.pdb(B-C)-19.1084688-292.962528IDAN.pdb(A-B)-614.082313-708.164873IDCP.pdb(A-B)-614.082313-708.164873	1BAM.pdb	(A-B)	0	-197.68285
1BFT.pdb-64.198907-361.3627171BIF.pdb(A-B)-67.565202-358.3354421BJ1.pdb(C-D)-279.688013-717.1241531BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-95.441015-424.0143751CG1.pdb(A-B)-95.441015-424.0143751CC2.pdb(A-B)-290.002746-589.7877261CS2.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-449.62655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1BCR.pdb	(B-A)	-1498.349104	-2061.407004
IBIF.pdb(A-B)-67.565202-358.335442IBJ1.pdb(C-D)-279.688013-717.124153IBRS.pdb(A-D)-625.16209-980.637IBSR.pdb(A-B)-791.959222-673.003592IBTH.pdb(A-B)-250.227808169.819502IBXG.pdb(A-B)-363.305094-668.539914IC1Y.pdb(A-B)-361.532653-617.980673ICC.pdb(A-B)-1277.646318-2480.783408ICC1.pdb(A-B)-57.505316-177.596316ICG2.pdb(A-B)-95.441015-424.014375ICHO.pdb(C-D)-151.052859-306.161859ICOZ.pdb(A-B)-290.002746-589.787726ICSE.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.6655-649.222415IDZJ.pdb(A-B)-489.626655-649.222415IDZ2.pdb(A-B)-489.62655-649.222415IDZ2.pdb(A-B)-411.414308-653.800728IDAN.pdb(B-C)-191.084688-292.962528IDBF.pdb(A-B)-614.082313-708.164873IDCP.pdb(A-B)-395.754696-594.116286	1BFT.pdb	(A-B)	-64.198907	-361.362717
IBJ1.pdb(C-D)-279.688013-717.124153IBRS.pdb(A-D)-625.16209-980.637IBSR.pdb(A-B)-791.959222-673.003592IBTH.pdb(A-B)-250.227808169.819502IBXG.pdb(A-B)-363.305094-668.539914IC1Y.pdb(A-B)-361.532653-617.980673ICDC.pdb(A-B)-1277.646318-2480.783408ICDT.pdb(A-B)-57.505316-177.596316ICG2.pdb(A-B)-95.441015-424.014375ICG1.pdb(C-D)-151.052859-306.161859ICO2.pdb(A-B)-290.002746-589.787726ICSE.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.693309-703.561989ICZJ.pdb(A-B)-448.6655-649.222415ID22.pdb(A-B)-411.414308-653.800728IDAN.pdb(B-C)-191.084688-292.962528IDBF.pdb(A-B)-614.082313-708.164873IDCP.pdb(A-B)-395.754696-594.116286	1BIF.pdb	(A-B)	-67.565202	-358.335442
1BRS.pdb(A-D)-625.16209-980.6371BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CG1.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-44.243303-204.0052231CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-B)-489.626655-649.224151D2Z.pdb(A-B)-489.626655-649.224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-395.754696-594.116286	1BJ1.pdb	(C-D)	-279.688013	-717.124153
1BSR.pdb(A-B)-791.959222-673.0035921BTH.pdb(A-B)-250.227808169.8195021BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-95.441015-424.0143751CG1.pdb(A-B)-95.441015-424.0143751CH0.pdb(C-D)-151.052859-306.1618591CO2.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-449.626655-649.2224151D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1BRS.pdb	(A-D)	-625.16209	-980.637
1BTH.pdb-250.227808169.8195021BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CH0.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-448.6557-459.6708271D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-395.754696-594.116286	1BSR.pdb	(A-B)	-791.959222	-673.003592
1BXG.pdb(A-B)-363.305094-668.5399141C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-442.24303-204.0052231CZY.pdb(A-B)-449.626655-649.2224151D2V.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1BTH.pdb	(A-B)	-250.227808	169.819502
1C1Y.pdb(A-B)-361.532653-617.9806731CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-B)-489.626655-649.2224151D2V.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1BXG.pdb	(A-B)	-363.305094	-668.539914
1CDC.pdb(A-B)-1277.646318-2480.7834081CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CH0.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-411.414308-653.8007281D2Z.pdb(A-B)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1C1Y.pdb	(A-B)	-361.532653	-617.980673
1CDT.pdb(A-B)-57.505316-177.5963161CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CH0.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-449.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CDC.pdb	(A-B)	-1277.646318	-2480.783408
1CG2.pdb(A-B)-80.239687-135.6348771CGI.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-449.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CDT.pdb	(A-B)	-57.505316	-177.596316
1CGI.pdb(A-B)-95.441015-424.0143751CHO.pdb(C-D)-151.052859-306.1618591CoZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-441.414308-653.8007281D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CG2.pdb	(A-B)	-80.239687	-135.634877
1CHO.pdb(C-D)-151.052859-306.1618591COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-449.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CGI.pdb	(A-B)	-95.441015	-424.014375
1COZ.pdb(A-B)-290.002746-589.7877261CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-449.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CHO.pdb	(C-D)	-151.052859	-306.161859
1CSE.pdb(A-B)-448.693309-703.5619891CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1COZ.pdb	(A-B)	-290.002746	-589.787726
1CZJ.pdb(A-B)-44.243303-204.0052231CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CSE.pdb	(A-B)	-448.693309	-703.561989
1CZY.pdb(A-D)-316.875657-459.6708271D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CZJ.pdb	(A-B)	-44.243303	-204.005223
1D2V.pdb(A-B)-489.626655-649.2224151D2Z.pdb(A-B)-411.414308-653.8007281DAN.pdb(B-C)-191.084688-292.9625281DBF.pdb(A-B)-614.082313-708.1648731DCP.pdb(A-B)-395.754696-594.116286	1CZY.pdb	(A-D)	-316.875657	-459.670827
1D2Z.pdb (A-B)-411.414308-653.8007281DAN.pdb (B-C)-191.084688-292.9625281DBF.pdb (A-B)-614.082313-708.1648731DCP.pdb (A-B)-395.754696-594.116286	1D2V.pdb	(A-B)	-489.626655	-649.222415
1DAN.pdb (B-C)-191.084688-292.9625281DBF.pdb (A-B)-614.082313-708.1648731DCP.pdb (A-B)-395.754696-594.116286	1D2Z.pdb	(A-B)	-411.414308	-653.800728
1DBF.pdb (A-B) -614.082313 -708.164873 1DCP.pdb (A-B) -395.754696 -594.116286	1DAN pdb	(B-C)	-191.084688	-292-962528
1DCP.pdb (A-B) -395.754696 -594.116286	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-C)	-177-319663	-286-224353
1DCP.pdb (A-D) -115.598403 -206.225183	1DCP.pdb	(A-D)	-115-598403	-206-225183
1DCP.pdb $(A-E)$ -57.09732 -94.69483	1DCP.pdb	(A-E)	-57.09732	-94.69483

1DEL ndb	(A-B)	-162 948465	-367 311505
1DEI odb	$(\Lambda - B)$	_20 022070	-256 626070
1 DEN - alla	(A-B)	-20.023078	-330.020070
IDEN.pab	(A-B)	-54.968686	-103.9/0080
IDHK.pdb	(A-B)	-5/1.5/2218	-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	$(\Delta - B)$	-229 758568	-404 906098
1E90.pub	$(\Lambda - B)$	0	-140 19966
1E90.pub	(A-B)		-140.10900
1EAI.pub	(A-C)	145 026404	-203.559202
1EFN.pab	(A-B)	-145.036484	-392.285414
lEFU.pdb	(A-B)	-661.3/34/6	-1223./46256
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
1FTP.pdb	(A-B)	-397.972495	-905.188485
1FLE pdb	(A-B)	-430 353724	-735 972914
1FM0 pdb	(A - B)	-531 /2/237	-820 844077
1 FNS pdb	(A D) (P_C)	-200 162516	-510 005106
1EC1 pdb		201 170502	- J40.00 J100
16CN mall	(A-B)	-201.179592	-441.060092
166N.pdb	(A-B)	-123.322095	-508.446005
1GG2.pab	(A-B)	-268.313504	-6/2.221664
lGL1.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
1 HWG. pdb	(A-B)	-271-267588	-683.078288
1TOH pdb	(A-B)	-422 774472	-699 594432
1 I CW pdb	$(\Delta - B)$	-317 894074	-616 047474
1 TUE pdb	(A D) (B-A)	-1028 903261	-17/2 /67271
1 TOT pdb	(D-A)	254 620601	-1/42.40/2/1
1 JDL pdb	(A-B)	-254.620691	-313.401391
	(A-C)	-440.38926	-808.56322
IJDH.pdb	(A-B)	-966./8//41	-154/.192551
lJDP.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
1K90.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
- <u>-</u>	· · · /		

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
1LOV.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 ndh	$(\Delta - B)$	-361 798828	-667 879608
1MEL pdb	$(\Delta - I_{\perp})$	-43 117137	-287 230847
1MJH pdb	$(\Delta - B)$	-441 888869	-714 984129
1MKA ndh	$(\Delta - B)$	-963 400669	-1548 096429
1MLC pdb	(A D) (B-F)	-121 0/3357	-328 698697
1MCD pdb		-52 222001	-212 700011
1M7W pdb	(A-B)		-212.700011
1MCA pdb	(A-B)	2 402011	105 251021
1NE2 malb	(A-B)	-3.402011	-105.251021
	(A-C)	-646.068039	-980.921579
INLU.pap	(B-C)	-202.8/966/	-336.960397
INMB.pab	(A-C)	-45.902415	-138.046455
10CU.pdb	(A-B)	-201.2602	-451.39942
10EB.pdb	(A-D)	-368.622501	-635.149751
10EY.pdb	(A-J)	-412.583004	-678.953074
10PH.pdb	(A-B)	-328.561635	-604.695645
10RY.pdb	(A-B)	-261.22928	-845.49114
10SP.pdb	(A-C)	-13.425325	-80.565475
10TF.pdb	(A-C)	-59.793689	-235.007439
10TF.pdb	(A-D)	-68.795105	-304.560795
10TF.pdb	(A-E)	-50.421502	-215.890832
10TG.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
101S.pdb	(B-C)	-418.711621	-730.126451
10DL.pdb	(B-A)	-129.066838	-510.849448
10DN.pdb	(A-B)	-423.894892	-579.590802
10FX.pdb	(A-B)	-1738.326431	-2640.313551
10H4 pdb	(A-B)	-1873 741736	-2548 793076
10KS pdb	(A-B)	-1861 665779	-2253 464519
1096 ndb	$(\mathbf{C} - \mathbf{E})$	-680 694476	-1008 026086
10SG ndb	(G-E)	-159 451131	-341 812121
1056 pdb	(G-H)	-622 108086	-1328 226376
100V ndh	(G-11) (A D)	-022.100000 572.95056	1100 5460
1017.pub	(A-B)	-572.05050 FC4 702124	-1190.J409 010 750424
1RUR.pub	(A-B)	-504.705124	-019.759424
IDEC	(A - C)	-201.004433 -207 065240	-430.929139 -440 210270
INEG.POD			-440.ZIU3/9
IREW.pap			-010.04922
1883.pdb	(A-B)	-143.42//96	-00/./69826
1KPU.pdb	(A-B)	U E O O O O O O O O O O O O O O O O O O O	-293.42267
IKYP.pdb	$(\perp - \perp)$	-598.00/345	-1048.850965
IKYP.pdb		-207.932592	-421.883692
1RYP.pdb	(⊥−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
1SO2.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
1TOF.pdb	(A-C)	-515.972008	-959.595988
1TOJ.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
1T02 pdb	(A - B)	-666 870096	-976 906126
1TTW pdb	$(\Delta - B)$	0	-112 09
1TW.pub	(A - B)	-393 302921	-577 256381
1TVX.pdb	$(\mathbf{R} - \mathbf{C})$	-194 77552	-208 91162
1TVA.pub	$(\mathbf{A} - \mathbf{B})$	-822 566878	-1210 538268
1TX4.pub	(A - B)	0	7 20/913
1114.pub		-1590 000/88	-1919 325239
1005.pdb	(A - I)	-5 761313	-1010.525250
1U8T ndb	(A-B) (A-F)	-144 826431	-209.559095 -311 537111
1UAD pdb	(A-C)	-287 329618	-518 5/0108
1UI7 pdb	(A-C)	-206 754075	-624 076615
1USZ.pub	(A-D) (A-D)	-442 000120	-609 912900
1US7.pub	(A-D) (A-D)	-522 564479	-010.013009
1USU.pub		-522.504478	1600 05550
1VE6 pdb	(A-B)	-75 194205	-405 403455
1VED odb		256 470170	403.403433
1VPD rdb		194 706742	-447.032119
1WDC pdb		220 572450	900 502150
1WDC.pdb	(A-B)	-239.373439	-009.000109
1WDC.pdb	(A-C)	-414.234024	-1031.002434
1WMH.pub	(A-B)	107 055011	1012 500001
1WMI.pdb	(A-B)	100 212072	-1013.300001
	(A-B)	-100.213873	-325.484753
1VC2 rdb		750 007654	-290.004300
1XGZ.pdb	(A-B)	-/59.89/654	-1028.255624
	(D-E)	-130.043/39	323.88363L
1YCS.pdb	(A-B)	-19/.18/166	-506.5081/6
1YDR.pdb	(A-B)	-294.907279	-/16.991589
	(А-В) (Р. С)	-8U/.3UI23	-1300.42433
		-332.9/4109	-339.04/129
	(A-B)		-342.200280
	(A-B)		-/51.322595
	(A-B)	-104.24/264	-82.151554
	(A-B)	-21/.2/6/89	-442.2/01/9
	(A-B)	-204.991195	-931.140895
∠GN5.pdb	(A-B)	U	0.44331

2HDH.pdb	(A-B)
2JEL.pdb	(B-C)
2KAT ndh	(B-T)
2000	
20HX.pab	(A-B)
20R1.pdb	(L-R)
20Z9.pdb	(A-B)
2PCC.pdb	(A-B)
2 PCH. pdb	(A-B)
2PRC ndh	(B-C)
2DTC rodb	
2PIC.pub	(A-B)
2RHE.pdb	(A-B)
2RUS.pdb	(A-B)
2SIC.pdb	(A-B)
2SNI.pdb	(A-B)
2SOD.pdb	(C-D)
2SPC.pdb	(A-B)
2TCT.pdb	(A-B)
2TEC.pdb	(A-B)
2THT pdb	(A-B)
2TMK pdb	(A - B)
2TMR.pub	(A = B)
2TRC pdb	(A - C)
2TRC.pub	(A C)
2151.pub	(A-B)
215C.pub	(A-B)
3ENL.pap	(A-B)
3FAP.pdb	(A-B)
3GRS.pdb	(A-B)
3ICD.pdb	(A-B)
3NOS.pdb	(A-B)
3PVI.pdb	(A-B)
3SDH.pdb	(A-B)
3SDP.pdb	(A-B)
3SGB.pdb	(A-B)
3SSI.pdb	(A-B)
3TPT pdb	(A-B)
4HTC pdb	(B-C)
4MDH ndh	(A-B)
5HVP ndb	(A-B)
6GSV ndh	$(\Delta - B)$
GDIV pdb	
okry.bap	(A-B)

-730.516022	-1171.869902
-285.907811	-420.578471
-55.968261	-245.229261
-1226.794268	-1735.094258
-30.210904	-114.714654
-345.773095	-782.369755
-456.953126	-568.827516
-1556.261954	-2395.175734
-124.159932	-308.871152
-412.268143	-675.613903
-426.754326	-575.360326
-817.287715	-1661.273255
-465.62034	-718.88683
-239.993022	-510.344012
-46.415505	-243.275765
-303.617417	-1247.839477
0	-531.23087
-316.384601	-566.725721
0	-25.34322
-173.751082	-469.145692
-459.847923	-735.624553
-911.928854	-1737.150604
-72.595253	-400.438993
-844.971449	-1494.111809
-430.929972	-798.826972
-246.076069	-330.743839
-24.834058	-603.403948
-122.711993	-674.140023
-1270.944449	-2082.878779
-367.103287	-852.061737
-678.475905	-958.243425
-29.508741	-279.413761
-210.813983	-428.457953
0	-116.07727
-383.378496	-645.098086
-936.160607	-1484.771147
-790.227608	-1353.255288
-/64.099305	-1353.996995
-966.536884	-1546.266054
-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
1A27 ndb $(A-B)$	-45 873306	-497 093756
1A27 pdb $(A-D)$	-10 832955	-92 296155
$1\lambda^{2}C$ pdb $(\lambda - P)$	-34 862977	-165 /0/207
1 A A B	-74 386892	-173 007692
$1 \lambda 17 \text{ mdb} (\lambda D)$	25 171254	220 220524
1AA7.pub (A-b)		-329.320324
1ACB.pub (A-B)		-207.003303
AFW.pdb (A-B)	-107.21920	-000.17500
1AK4.pdb (A-C)		
IALK.pdb (A-B)	-164.075265	-1444.958855
IAUR.pdb (A-B)	-77.589086	-508.265196
IATL.pdb (A-B)	0	- /2.9/58/
IAVW.pdb (A-B)	-55.235941	-416.262671
IAY/.pdb (A-B)	-47.063512	-318.886032
1BON.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
1D27 pdb $(A-B)$	-46 883859	-289 246279
1DAN pdb (B-C)	-35 509187	-137 387027
1 DBF 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
1 DCP adb (A = D)	0.1000/0	- 20.012100
IDCF.PUD (A-E)	U	-3/.49UII

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
1DOI.pdb	(A-D)	-14.914089	-150.087509
1DS6.pdb	(A-B)	-41.375393	-376.531083
1DVF.pdb	(B-D)	-49.212778	-225.140388
1 DVJ, pdb	(A-B)	-12.07454	-58-4313
1DX5.pdb	(T-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
1EAV ndb	$(\Delta - C)$	-23 874601	-183 240051
1EFN pdb	$(\Delta - B)$	-17 226177	-264 475107
1FFU pdb	$(\Lambda - B)$	-97 289183	-658 739963
1Eru.pub	(A D) (A D)	-30 332603	-333 127173
1EWV.pub		144 56221	760 20162
1EUV.pub		-144.00001	
1EAI.pub	(A-B)	-40.03330	-525.14071
1F37.pdb	(A-B)	-24.901900	-2J2.10/290 527 045001
1F/4.pab	(A-C)	-30.557831	-53/.845881
1F9Z.pdb	(A-B)	-245.80708	-898.18312
lFDL.pdb		-24.481942	-98.263502
1FIN.pdb	(A-B)	-96.365953	-556.937693
lFlP.pdb	(A-B)	-93.095152	-600.311142
lf'LE.pdb	(A-B)	-69.61/1/2	-3/5.236362
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
1K90.pdb	(A-B)	-61.639662	-361.556692
1KB5.ndh	(В-Н)	-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
10C0.pdb (A-B)	-58.127641	-308.266861
10EB.pdb (A-D)	-30.215621	-296.239871
10EY.pdb (A-J)	-42.647712	-308.946782
10PH.pdb (A-B)	-81.504961	-357.638971
10RY.pdb (A-B)	-35.557761	-619.594621
10SP.pdb (A-C)	0	-67.14015
10TF.pdb (A-C)	-59.793689	-235.007439
10TF.pdb (A-D)	-68.795105	-304.560795
10TF.pdb (A-E)	-43.498236	-208.967566
10TG.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
IPP2.pdb (A-B)	-31.292664	-381.242234
IPPF.pdb (A-B)	-56.356729	-289.104789
IPYT.pdb (A-B)	- /6.52394 /	-402.949/0/
IPYT.pdb (B-D)	-24.398453	-164.813453
IQIS.pdb (B-C)	-107.059872	-41/.94//02
IQDL.pab (B-A)	-4/.11360/	-428.89621/
IQDN.pab (A-B)	-8./39835	-164.435/45
IQFX.pab (A-B)	-155.4/4/39	-105/.461859
1QH4.pab (A-B)	-157.602012	-832.033332
IQKS.pdb (A-B)	-182.537846	-5/4.336586
IVSG.pdb (G-E)	-52.191902	-30/.129392 -23/ 01521
10SC pdb (G-H)	-8/ 537116	-234.01331 -790 655/06
10TX pdb (A=B)	-04.00/110	-790.000400 -650 056107
$1 \mathbb{P}(\mathbb{R} \times \mathbb{P})$	-82 960704	-338 017004
1R3.1 ndb $(A-C)$	-33 48249	-188 5/715
$\frac{1}{1} \operatorname{REG} \operatorname{pdb} (A = B)$	-63 550381	_304 605511
$\frac{1}{1} \operatorname{REW} \operatorname{pdb} (R-D)$	-45 521732	-305 761997
1RP3 ndh (A-B)	-47 782273	-569 538303
TITTO-POD (A D)	11.102213	505.550505

1RP0.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
1SO2.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
1TOF pdb	(2 - C)	-67 682725	-511 306705
1TOL pdb	(B-C)	0	-218 02265
1TA3 pdb	(A-B)	-19 773159	-269 611609
1TAB pdb	(A-B)	-47 144988	-252 285628
1TAW pdb	$(\Delta - B)$	-63 200492	-343 762142
1TC1 pdb	$(\Delta - B)$	-73 075715	-545 787515
1TCS pdb	(A - B)	-8/ 218113	-383 735/93
1TO2 pdb	(A - B)	-78 735322	-388 768352
1 TTW pdb	(A - B)	0	-112 084
1TW.pub	(A-B)	-67 347872	-112.004
1TVX.pub	$(\mathbf{R} - \mathbf{C})$	0	-231.300332
1TVA.pub	$(\mathbf{D} - \mathbf{C})$	-55 72/998	-14.1301
1TX4.pub	(A - B)	0	7 20/913
1119.pub	$(\Lambda - \Sigma)$	-12 383116	-240 703866
1003.pdb	(A - I)	-12.303110	-240.703000
100n.pub	(A-B)		-200.993093
1001.pdb	(A-C)	-70 186224	-220.110025
10AD.pub	(A-C)	-62 450145	-201 672605
1002.pdb	(A-D)	-42 120692	-301.072003
1US7.pub	(A-B)	-42.130003	-207.033303
1050.pdb	(A-D)	-00.090704	1600 95550
101G.pdb	(A-B)	-40 232451	_270 101511
1VED pdb		20 207024	121 620074
IVFB.pdb		-30.28/034	-121.639974
1WDC malb	(A-C)	-85.060612	-377.582102
1WDC.pdb	(A-B)	-66.798824	-636.665524
1WDC.pdb	(A-C)	-54.390909	-691.958519
1WMH.pab	(A-B)	-56.449234	-349.648594
IWMI.pdb	(A-B)	-187.055211	-1013.421801
1 WQJ.pab	(A-B)	-37.398089	-262.665969
1 WWW.pab		-22.292847	-IUI.99804/
IXG2.pdb	(A-B)		-313.184991
		-4J.6L93U/	414.908083
IYUS.pdb	(A-B)	-44.621/41	-353.942/51
TIDK.pdb		$-\delta \angle \cdot / \perp \delta \angle / 4$	-304.795584
1YPI.pdb	(A-B)	-11/./89068	-6/6.912148
110V.pdb		-42.831414	-228.9043/4
⊥Z/K.pdb	(A-B)	-/2.363152	-338.172322

-35.325674	-12.606464
0	-224.99339
-264.991195	-931.140895
0	0.44331
-36.681394	-478.035274
-11.350914	-146.021574
-55.968261	-245.229261
-90.893186	-599.193176
-28.03247	-112.53622
0	-436.59666
0	-111.85799
-168.993104	-1007.906884
-41.550097	-226.261317
-52.765907	-316.111667
-19.520738	-150.417688
-171.105421	-1015.090961
-83.770603	-337.037093
-71.766355	-342.093345
-46.415505	-242.210765
-67.926163	-1012.148223
0	-531.23087
-52.04928	-302.3824
0	-25.34322
-15.236656	-310.630266
-47.718816	-323.415446
-167.665323	-992.878073
-72.595253	-400.438993
-57.301303	-706.440663
-38.874989	-435.349589
-3.645412	-88.312482
-24.834058	-603.403948
-122.711993	-674.140023
-88.207786	-233.946316
-200.776286	-1012.710616
-70.349954	-555.308404
-36.260101	-316.027621
-10.77542	-260.68044
-68.229701	-285.873671
0	-116.07727
-57.843786	-319.563376
-16.289319	-181.209319
-104.942977	-653.323517
-97.057867	-660.085547
-185.859764	-774.112454
-29.128463	-608.857633
-66.652887	373.054273
	$\begin{array}{c} -35.325674\\ 0\\ -264.991195\\ 0\\ -36.681394\\ -11.350914\\ -55.968261\\ -90.893186\\ -28.03247\\ 0\\ 0\\ -168.993104\\ -41.550097\\ -52.765907\\ -19.520738\\ -171.105421\\ -83.770603\\ -71.766355\\ -46.415505\\ -67.926163\\ 0\\ -52.04928\\ 0\\ -15.236656\\ -47.718816\\ -167.665323\\ -72.595253\\ -57.301303\\ -38.874989\\ -3.645412\\ -24.834058\\ -122.711993\\ -88.207786\\ -200.776286\\ -70.349954\\ -36.260101\\ -10.77542\\ -68.229701\\ 0\\ -57.843786\\ -16.289319\\ -104.942977\\ -97.057867\\ -185.859764\\ -29.128463\\ -66.652887\\ \end{array}$