

Supporting information to: Unique Physicochemical Patterns of Residues in Protein-Protein Interfaces

Tamas Lazar^{1,2}, Mainak Guharoy^{1,2}, Eva Schad³, Peter Tompa^{1,2,3,}*

¹ VIB-VUB Center for Structural Biology, Vlaams Instituut voor Biotechnologie, Pleinlaan 2,
1050 Brussels, Belgium.

² Structural Biology Brussels, Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussels, Belgium.

³ Institute of Enzymology, Research Centre for Natural Sciences, Hungarian Academy of
Sciences, Magyar tudosok korutja 2, 1117 Budapest, Hungary.

* email address: peter.tompa@vub.be

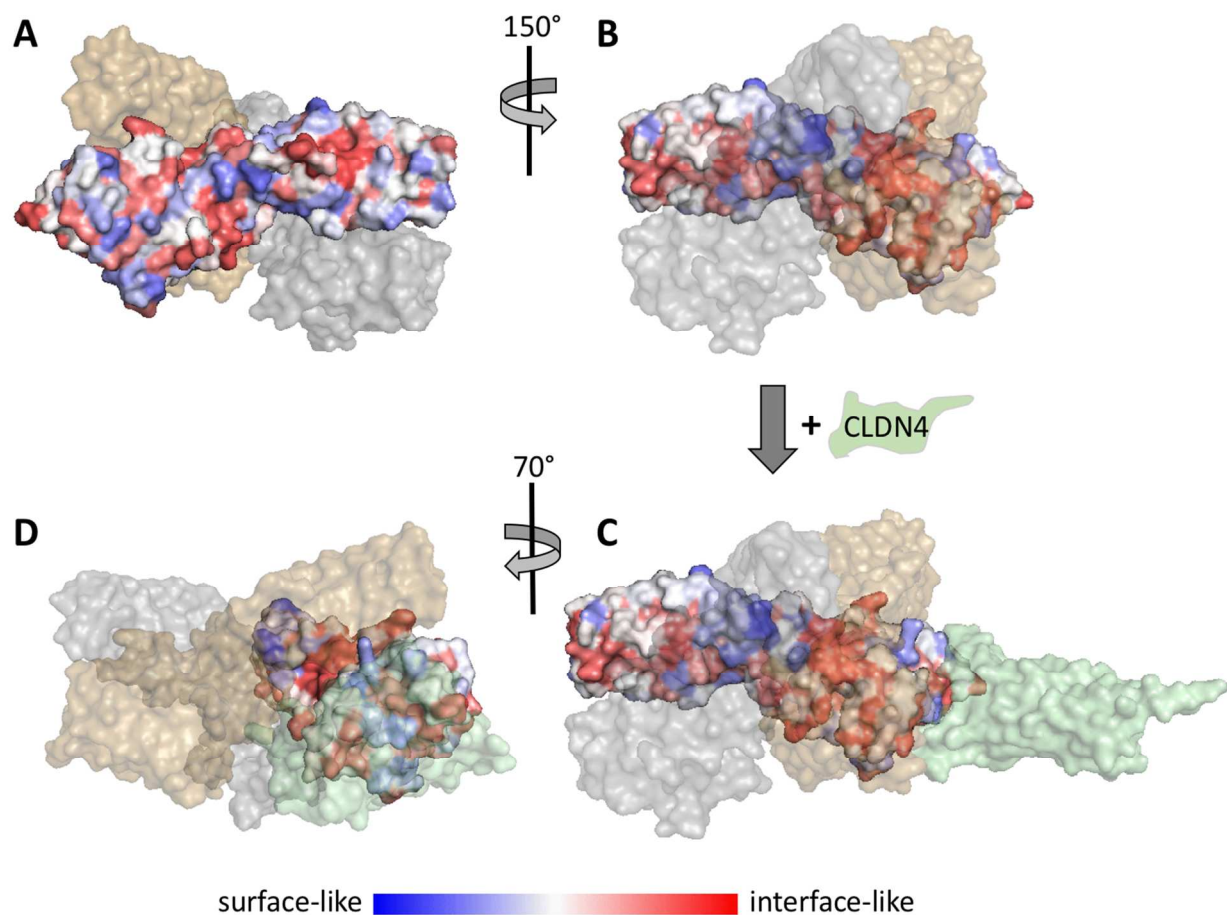


Figure S1. *Clostridium perfringens* enterotoxin trimer (PDB: 3ZIW) with the iPat scores projected onto the surface.

- A) iPat scores on the non-interface surface of an enterotoxin monomer.
- B) iPat captures the binding site of the golden colored monomer much better than of the silver colored.
- C) *C. perfringens* enterotoxin also forms complex with human Claudin-4 (PDB: 5B2G, colored by green).
- D) iPat scores of enterotoxin residues interfacing with Claudin-4.

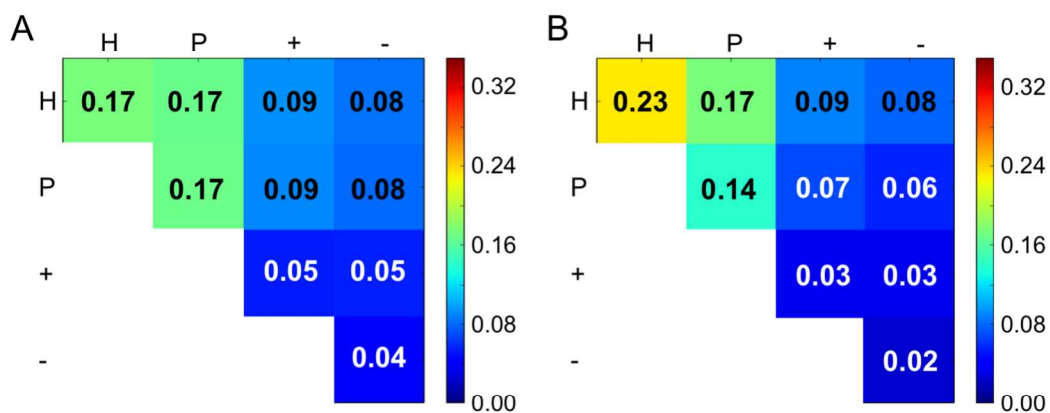


Figure S2. Heatmaps calculated for crystal packing dimers showing the frequencies of middle-range contacts between residues of different physical properties.

The frequencies of residues with each of the 4 physicochemical properties (H: hydrophobic, P: polar uncharged, +: positively charged, -: negatively charged) within the cutoff distance from central residues with a given property for the non-interacting surface residues (A) and interface core residues (B).

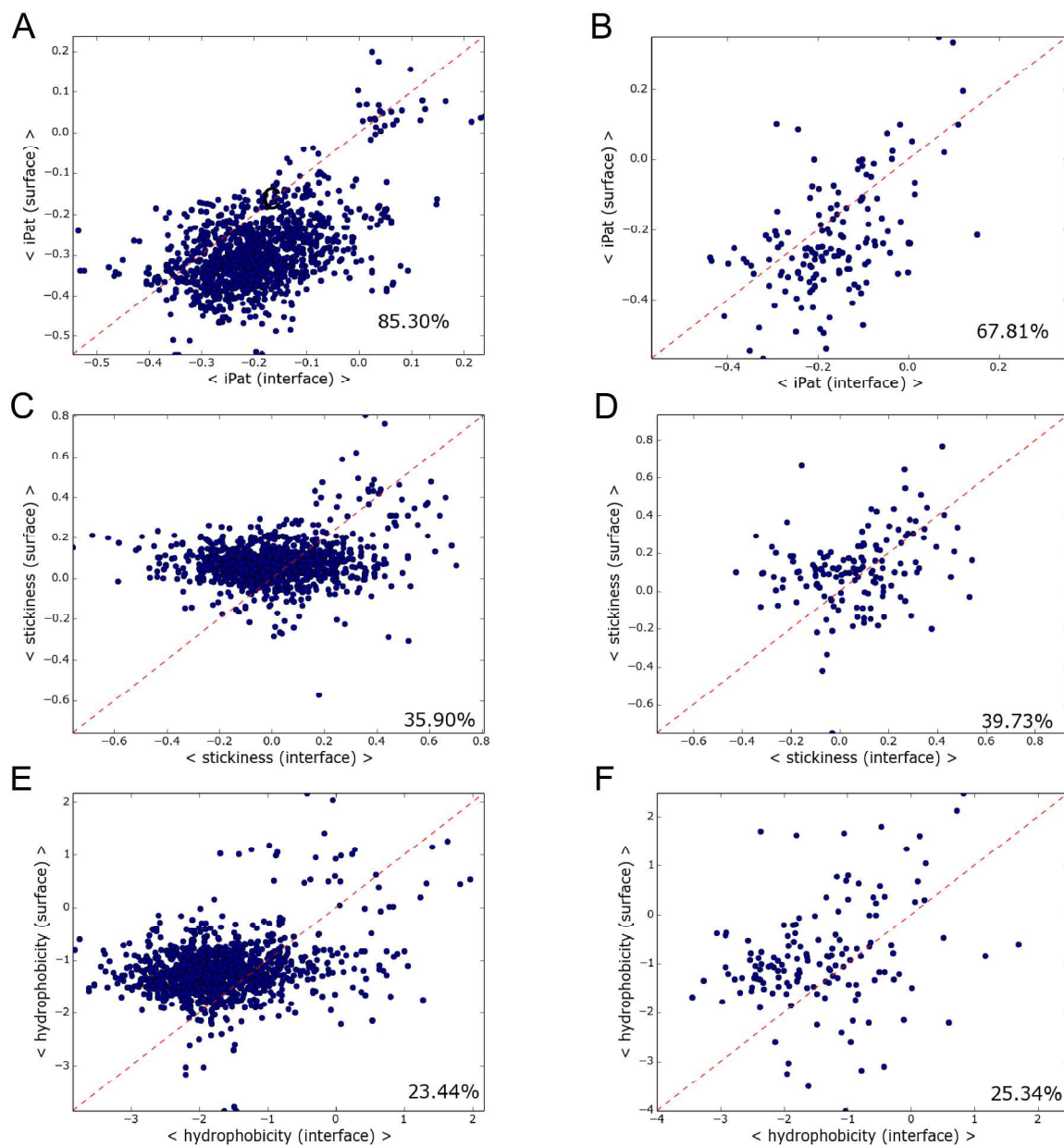


Figure S3. Scatter plots of average iPat, stickiness and hydrophobicity values for all interface residues (rim residues included) and non-binding surface residues in individual protein chains of the analyzed data sets.

A) Test set - iPat; B) Disordered protein/peptide set - iPat; C) Test set - stickiness; D) Disordered protein/peptide set - stickiness; E) Test set - hydrophobicity; F) Disordered protein/peptide set - hydrophobicity. For all complexes, we distinguished non-binding surface- and interface residues, and

determined their iPat and stickiness scores. For each protein, the average of scores of their non-binding surface vs. the average of scores of their interface residues was plotted. Interface residues (with the rim included), on average, have significantly higher iPat values than non-binding surface residues in both the test set (A) and the disordered protein/peptide set (B). In the test set 85.30% while in the disordered protein/peptide set 67.81% of the chains had higher iPat values for the interface than for the non-binding surface. The same is not true for stickiness and hydrophobicity (C-F), less than 40% of the chains had higher average stickiness values for the interface than for the non-binding surface in both datasets.

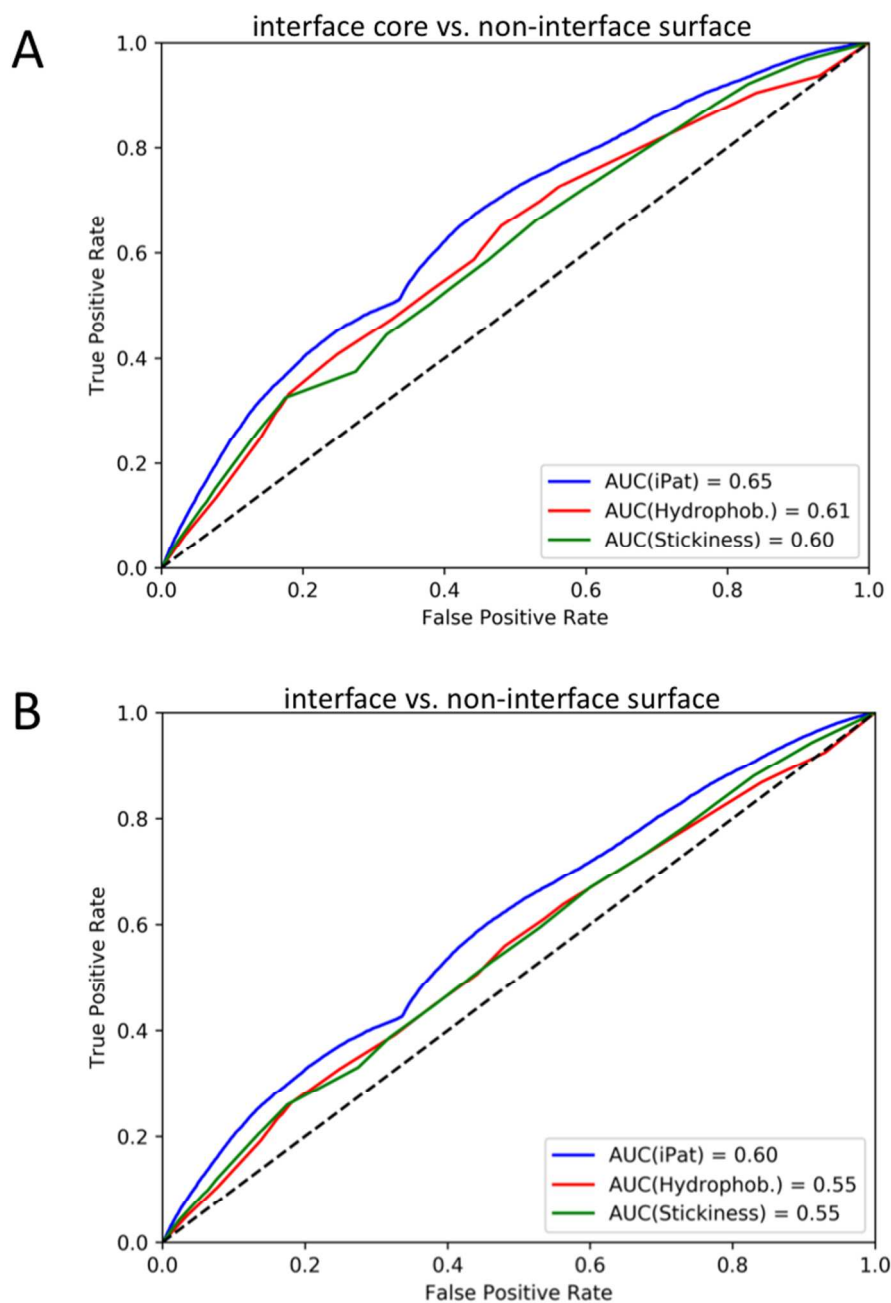


Figure S4. Receiver Operating Characteristic (ROC) analysis of iPat, hydrophobicity and stickiness on the test set.

A) ROC curves of the interface core vs. non-interface surface residue classification.

B) ROC curves of the interface vs. non-interface surface residue classification.

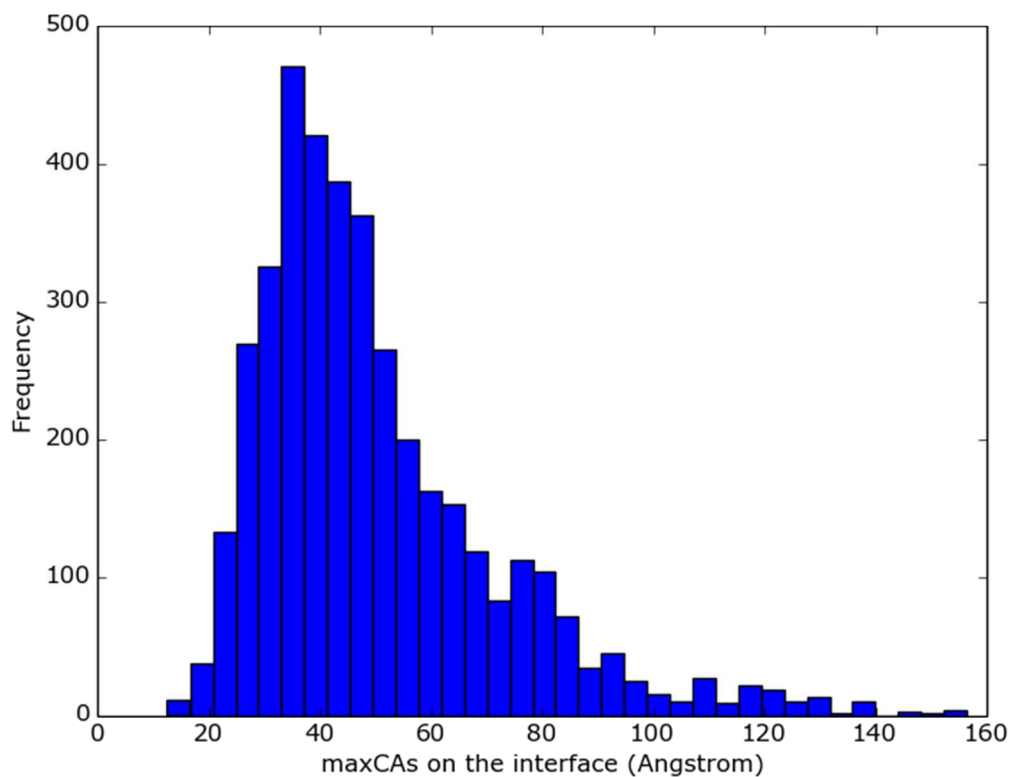


Figure S5. Frequency distribution of maximum C α -C α atom distances of interfaces in the training set.

The frequency of the maximum C α -C α distances for all complexes in the training set are plotted. The figure shows that the threshold of 12Å for patches is reasonable since even for the smallest interfaces multiple patches will contain the interface residues.

Table S1. Protein Data Bank identifiers of proteins in the data sets.

(A) Training set; (B) Test set; (C) Crystal contact set; (D) Disordered proteins set.

A) Training set									
1A0F	1MKK	1VKE	2E0A	2O99	2WLV	3CWF	3H86	3N01	3T9O
1A4P	1MOX	1VKH	2E65	2OAR	2WN2	3CXK	3H87	3N06	3TA6
1A92	1MR1	1VL0	2E6E	2OB3	2WQI	3CZ8	3HA2	3N08	3TD3
1AB8	1MVF	1VPM	2EB4	2OB9	2WTM	3CZQ	3HA4	3N1F	3TDQ
1AHS	1MWQ	1VQS	2EGI	2OCT	2WUJ	3D0F	3HE5	3N2N	3TEQ
1AOH	1MXR	1VR4	2EJ8	2OD4	2WUQ	3D0T	3HEI	3N4R	3TGN
1APY	1MY7	1VR7	2F0X	2ODK	2WX3	3D36	3HF5	3N65	3TJ8
1AY7	1N1J	1VRA	2F22	2ODM	2WY3	3D3B	3HFO	3N8B	3TLO
1AYF	1N5B	1W23	2F4M	2OFC	2WY7	3D3S	3HHT	3N9S	3TMP
1B2P	1N8K	1W5M	2F5K	2OIE	2WYT	3D55	3HHW	3NBC	3TQN
1B5F	1NC7	1W98	2F6M	2OIK	2WZ1	3D5R	3HIA	3NHE	3TR3
1B93	1ND6	1W9A	2F6U	2OJ6	2WZ7	3D8L	3HIE	3NI0	3TRT
1BD3	1NHG	1WMG	2F86	2OKU	2X2V	3D9X	3HIM	3NJC	3TUO
1BH8	1NLQ	1WMX	2F9H	2OMO	2X36	3DA0	3HLS	3NJR	3TXS
1BKJ	1NR4	1WNR	2FA5	2OOI	2X9A	3DAQ	3HLX	3NKH	3UID
1BP3	1NWW	1WOC	2FA8	2OPI	2X9G	3DCA	3HTN	3NKL	3UIU

1BTE	1NX4	1WP8	2FCW	2OT4	2XDG	3DDC	3HVZ	3NNQ	3U22
1BTK	1NXM	1WQ6	2FDB	2OX7	2XHF	3DDT	3HX8	3NO6	3U43
1BWO	1NZI	1WQJ	2FHZ	2OXG	2XIU	3DDV	3HXF	3NPF	3U7I
1C28	1O5E	1WT6	2FIP	2OXL	2XIW	3DF6	3HXJ	3NRP	3U80
1C41	1O6A	1WTH	2FIU	2OY9	2XME	3DFE	3I4Z	3NTV	3UB6
1C4Q	1O7Z	1WWR	2FJC	2P04	2XMJ	3DHX	3I96	3NV0	3UCA
1C5E	1O9R	1X2I	2FOM	2P06	2XOL	3DHZ	3I9F	3NYB	3UFE
1C6V	1OJH	1X6I	2FPE	2P0A	2XTC	3DI2	3IBW	3O1N	3UKN
1CI4	1ONK	1X8D	2FQM	2P13	2XTS	3DLQ	3IC3	3O21	3ULB
1CI6	1OR7	1XBY	2FS2	2P1B	2XTY	3DN7	3ICA	3O27	3UUW
1CKS	1ORY	1XD3	2FTX	2P1M	2XU6	3DPL	3ICX	3O2I	3UWL
1CNT	1OSY	1XDT	2FUR	2P5M	2XU8	3DQG	3IF4	3O5W	3UWS
1CPC	1OU0	1XFF	2FZV	2P63	2XVO	3DR4	3IFQ	3O6Q	3UZQ
1CQK	1OUW	1XG2	2G2N	2P7O	2XVT	3DRZ	3IIC	3O6Z	3V2U
1D0D	1P6O	1XIL	2G4C	2P7V	2XZ8	3DSB	3ILW	3O8E	3V4H
1D2O	1PJH	1XK4	2G84	2P8I	2Y1T	3DSS	3IMA	3O8Q	3V4K
1D3B	1PKV	1XL3	2GAO	2PBQ	2Y3N	3DUH	3IPR	3O94	3V4Y
1D9C	1PM3	1XLY	2GEC	2PDO	2Y43	3DWA	3IUW	3OA2	3V5R
1DKG	1PM4	1XQA	2GEY	2PEI	2Y4Y	3DXR	3IWF	3OAM	3V67

1DOK	1PN4	1XSQ	2GF4	2PF4	2Y8C	3DZZ	3JTH	3OE3	3V69
1DTD	1PQH	1XTG	2GFQ	2PFW	2Y8N	3E10	3JVO	3OEO	3VBJ
1EAI	1PSR	1XU9	2GHJ	2PKD	2Y9M	3E19	3JXO	3OF5	3VCX
1EAJ	1PTM	1XVS	2GHV	2PMU	2YAD	3E1E	3K0L	3OFG	3VEJ
1EDY	1PUG	1Y66	2GIA	2PNZ	2YDA	3E48	3K1E	3OGH	3VEM
1ETX	1PXV	1Y6Z	2GIB	2PQR	2YFA	3E5U	3K1R	3OGI	3VIQ
1EUV	1PYA	1Y7R	2GIX	2PTT	2YH9	3E7K	3K2Y	3OGP	3VMX
1EXT	1Q08	1YA5	2GJ3	2PYB	2YHO	3E7L	3K3C	3OHE	3VP9
1EZG	1Q23	1YCY	2GLZ	2PZH	2YVE	3E7N	3K67	3OII	3ZQM
1F08	1Q40	1YJ7	2GM8	2PZZ	2YVR	3E8O	3K7U	3OJ6	3ZRG
1F3U	1Q4U	1YSJ	2GMY	2Q0S	2YWW	3E95	3KA5	3OKX	3ZRX
1F86	1Q5Y	1YUM	2GPE	2Q2I	2Z26	3EAB	3KAL	3OL3	3ZW5
1FC3	1Q67	1YUZ	2GRE	2Q30	2Z2S	3EGG	3KAV	3OLJ	3ZWF
1FD3	1Q7L	1YXB	2GSL	2Q5W	2Z3Q	3EGR	3KBH	3ONR	3ZWH
1FE0	1QB5	1YYV	2GSV	2Q8V	2Z57	3EIK	3KCU	3OOV	3ZXC
1FLT	1QGK	1Z3E	2GTR	2QA7	2Z5B	3EJ3	3KE7	3OQP	3ZXO
1FM0	1QOP	1Z84	2GU9	2QAZ	2Z5I	3EJ9	3KF6	3OSS	3ZY7
1FR3	1QOU	1Z8H	2GUK	2QE8	2Z7F	3ELK	3KF8	3OUT	3ZYI
1FS1	1QSD	1ZBX	2GUM	2QE9	2ZCM	3EMF	3KGK	3P04	3ZZS

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1FYH	1QX4	1ZOQ	2GZ4	2QIF	2ZFD	3ERM	3KJJ	3P5T	4A5N
1G1C	1QYN	1ZOW	2H1E	2QJV	2ZGL	3ES4	3KM3	3P73	4A5U
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1GD9	1R8H	1ZV1	2H98	2QS7	2ZUG	3EW0	3KOP	3PGG	4AB0
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1GO4	1S28	2A5Y	2HJ9	2R2C	3A2V	3F2I	3KU7	3PM7	4AXO
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1H41	1SQS	2AO9	2HZ5	2RBB	3AKL	3FAU	3KYS	3Q7R	4DHI
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1I85	1TBX	2B1X	2IA1	2UUY	3B4R	3FJU	3LHK	3R0A	4EDH
1IAR	1TC1	2B5L	2IA9	2UUZ	3B4S	3FKA	3LHQ	3R24	4EGU
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1JBM	1TZP	2BMO	2IML	2V6K	3BE8	3FT7	3LSG	3RHI	4EVY
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1JS1	1UF5	2CAR	2J98	2VHA	3BT3	3G46	3LYN	3RRI	4FEE
1JYO	1UFI	2CG9	2J9U	2VJE	3BU2	3G4E	3LYX	3RWN	4FMH
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1KZA	1UNG	2CLB	2JD3	2VLQ	3C2U	3G8K	3M8E	3S5B	4G27
1KZQ	1UPT	2CO7	2JDQ	2VN5	3C5O	3GAE	3M8J	3S81	4G7N
1KZU	1US6	2CPG	2JER	2VS0	3C5X	3GCG	3M92	3S8I	4G7X

1KZY	1US7	2CU3	2JGS	2VSH	3C6V	3GDM	3MA2	3S8K	4G8S
1L2W	1USC	2CVI	2JK3	2VSM	3C8L	3GIU	3MAY	3S9D	4GEK
1L6R	1USL	2CZD	2JKH	2VWV	3CC9	3GIX	3MB2	3SF4	4GHG
1LDD	1UTY	2D0O	2JLM	2VX8	3CHB	3GLA	3MCB	3SF5	4GI3
1LGH	1UUI	2D2A	2NLV	2W1V	3CI5	3GLV	3MFX	3SHG	4GIP
1LJ7	1UUZ	2D5K	2NPT	2W2G	3CI9	3GMX	3MGJ	3SJR	4GJT
1LKT	1UV7	2D7E	2NQD	2W4L	3CJH	3GRD	3MJD	3SK2	4GO6
1LPB	1UZ3	2DC3	2NR5	2W4S	3CJS	3GWL	3MJG	3SLZ	4GSK
1LQK	1V0Z	2DFX	2NVA	2W6A	3CL3	3GWN	3MK6	3SOZ	4GVQ
1LUC	1V8H	2DJ6	2NVM	2W7R	3CLK	3GYG	3ML1	3SSA	4GYM
1LVW	1V8Q	2DJL	2NXV	2W7Z	3CNV	3GZ7	3MM5	3SSS	4GZR
1LYL	1V9D	2DLB	2O23	2W82	3COL	3GZA	3MMH	3SWY	4GZV
1M1E	1V9Y	2DOQ	2O27	2W8M	3CP7	3H05	3MMY	3SXX	4H41
1M1F	1VDR	2DPL	2O2A	2W8X	3CR3	3H3H	3MOL	3SZH	4H6C
1M1N	1VF6	2DQR	2O30	2WAS	3CS5	3H3M	3MQH	3T63	4H7P
1M2D	1VH5	2DRE	2O35	2WBV	3CT6	3H43	3MSU	3T6O	4HEC
1M44	1VIO	2DRV	2O38	2WIQ	3CT9	3H5N	3MSX	3T7Y	4HKI
1MFT	1VJH	2DS5	2O5H	2WJ9	3CTP	3H6P	3MW6	3T8K	4SGB
1MG7	1VJQ	2DSY	2O8A	2WJV	3CU2	3H7A	3MZ2	3T97	7AHL

1MJU	1VK8	2DVW	2O8X	2WKB	3CVJ	3H7H			
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B) Test set									
4ZB1	4WGF	4BHU	4WBA	4UG1	4Q1T	4LQK	4R7Y	4EGT	3WO5
4TNP	4OK9	4U5H	4CN1	4COF	4JAT	4RG2	3WJA	5CM6	4CFG
4G51	4IYQ	4YP5	4KH6	5IDY	4TU1	3WSJ	3VP6	4V2P	5CGL
4QAA	4IIB	4L37	5I5M	4ISD	4MI1	4JPH	3X1B	4KQW	4NLJ
4RXF	4AV7	4KQM	4K9Q	4CLC	4NY0	4XRN	4CRT	3WZZ	5CQE
4UUI	5CVJ	4P07	4ADG	4CL6	4HKT	4IP8	4P2L	4M8Z	4LOA
3WSE	4HZD	4IMA	3USF	4RFX	3ZJG	4FQN	4GA6	4UUY	4WH5
5BPS	4J4S	4OE5	5DEN	3V2R	4I4I	4OX0	4MFV	4ZNO	4JAK
4QII	4O4S	4KKZ	4GAE	4BQE	3W9B	5IE9	3V8D	4WJ0	4PIC
4R31	4OAK	4BOF	4YJY	4PFP	4RZ5	4RP3	4PLP	4P5W	4ON3
4RJ2	4L7B	3UVA	4C8R	4QC0	4XGV	4WAI	4D2I	4F8E	4MPM
4XRD	5HM8	4Q31	4FP1	4BAA	4OLC	3X38	4XCI	4AK9	3WMD
3WCT	4ZZ7	5CPL	4FJU	3WEZ	5EKE	4NC7	4FB8	5C1F	4YWZ
4D2E	4H80	4IWH	4E75	5CZK	4X04	4HFX	4QLA	4W8K	4HEQ
4HNZ	4NSL	4PMV	5AYD	4NA1	4IQD	4M3L	4FL0	4BNE	3TLD
4C2K	5IJZ	4W6Z	5AOW	4IA5	4LY4	4O0M	3ZHC	4MQ6	4OM7

4O48	4IL0	4GIU	4IGM	3ZO9	4Q5O	5I2M	4IX8	4I9A	3VV1
4L7Q	3ZDS	4ZGS	4LMA	4ZP1	4NDO	4UXE	4BWX	4RG1	4ZU5
3ZO8	4IDN	4UCG	4CCR	4WMJ	4MIK	5F1C	4DNX	5HSX	5C5Z
4TLX	4JEV	5HW0	3WMX	4DO3	4NSY	4X8I	4U7J	4KY9	4B54
5I5X	4DOY	4W9N	4L5Y	5A2G	4JUQ	5CVC	5HH3	4CWC	4Q77
5DND	4RAP	4OQN	4M1E	4TWA	4YAM	4R9O	4H0O	5DZS	4EHS
4YB6	5COB	4MRI	3VVK	4KPR	3WDK	4CQJ	5D3O	4O5F	4HZA
4KWH	3WIC	4OE7	3WOG	4L4L	5DLC	4E6T	4Y2W	5B0V	4OTN
2YNF	4D65	4XSL	4OQD	3WDP	4NEF	4X3N	4WD3	5CA5	4HKE
5DIB	5HWJ	4CMW	4ZM1	4N0B	5C0O	4QTN	3WCO	4ZLP	3V9M
4WZ5	3V0Q	5AVM	4F7O	5C2I	4WKB	4WIA	3ZPX	5F1R	4OTM
3WOM	4LIN	5EA2	4EDI	4KIR	4FE2	4NYT	4TR6	5DA1	4NLH
4BIM	3ZIW	4Z54	4PZA	4OHF	4OBW	4MYO	4O23	4IO1	4P1M
4O1Z	5HAC	4BYY	3WG9	4O7O	4GSN	4RV4	4TR7	4E9J	5B08
4UQV	4RPN	4KAS	4ZIL	4OKS	5AGY	4LCZ	4YSH	4TL3	4BK0
4C5J	3VDP	4WYV	4CO9	4R8F	4J91	4M99	4IZG	4IJ5	4KUN
4K3N	4JIT	4OFM	4E0F	4MZA	4O6Y	4UM4	4R8D	4UXU	4LID
4R88	4AL9	4XOM	4JE6	4HJ1	3ZFB	4U2U	4NSW	4FZS	4I6P
4YUV	4PHJ	4HS4	5CY4	4M9D	4I1V	5CMO	4UVJ	4NZY	4QNC

4ONC	4Q86	4QXP	4KYK	5HW2	4DF1	4CW9	4HNE	4CBP	4OIJ
4JLN	4KK0	4CPC	4M0K	4R7U	4QYT	4Q2P	4NQ3	4RHP	4PU7
4NAH	4LE5	5DZN	4MJ8	4XG1	4IT5	4V2O	5CRY	5HFK	4R3Q
4Q75	4I0U	4UC4	4URQ	4WJB	4ABX	4M8A	4KQK	4JYK	5A1Q
3WGO	4YJD	4Y89	4BMG	4K0B	4CS8	4WD9	4PVC	4P3F	4FDX
4MQR	4IS4	4CHK	4NHF	4I8A	4PXT	3ZGB	4O1L	4KGH	4W7Y
3WT4	4Z90	5CJ1	3VB2	4M3P	3WMU	4KTP	4ILK	4HUT	4DCZ
5BPF	4P2V	4LL7	4LKB	3WY7	4K30	4Q1V	4HFJ	4P0U	4GKG
3WWP	5C6M	4N1J	4OZN	4U83	4HBL	3WKY	2YQ2	4Q9V	4J8C
4UV2	4PZU	5DO6	4NKN	5CTO	3WU0	4IST	3WLX	4U9N	2YMY
4PZL	4BEM	4W7P	4Y6I	4KLA					

C) Crystal contacts (with the origin of the data)									
1A12	Bahadur	1DSU	Bahadur	1MWC	Bahadur	2BLS	Bahadur	1J96	DCXtal
13PK	Bahadur	1DXM	Bahadur	1NAW	Bahadur	2G3P	Bahadur	1LQT	DCXtal
1A3Y	Bahadur	1DYS	Bahadur	1NMT	Bahadur	2J5X (1HFV)	Bahadur	1N45	DCXtal
1A7T	Bahadur	1DZ4	Bahadur	1OME	Bahadur	2SCP	Bahadur	1PP3	DCXtal
1A7V	Bahadur	1EHY	Bahadur	1OVW	Bahadur	2SHP	Bahadur	1UEB	DCXtal
1AD5	Bahadur	1ELP	Bahadur	1PVA	Bahadur	2TPS	Bahadur	1VQQ	DCXtal

1AE9	Bahadur	1EPA	Bahadur	1QCI	Bahadur	2UGI	Bahadur	1YNQ	DCXtal
1AFK	Bahadur	1FGK	Bahadur	1QDM	Bahadur	3NG1	Bahadur	1ZLQ	DCXtal
1AG9	Bahadur	1FJM	Bahadur	1QHA	Bahadur	3PMG	Bahadur	2CKI	DCXtal
1AJK	Bahadur	1FMT	Bahadur	1QPA	Bahadur	5TSS	Bahadur	2E1V	DCXtal
1AMU	Bahadur	1FVK	Bahadur	1RB3	Bahadur	830C	Bahadur	2F37	DCXtal
1AQ0	Bahadur	1G2A	Bahadur	1RGE	Bahadur			2GAS	DCXtal
1AQZ	Bahadur	1GAR	Bahadur	1SHK	Bahadur			2J46	DCXtal
1ATL	Bahadur	1HRN	Bahadur	1SW6	Bahadur			2Q7D	DCXtal
1AW7	Bahadur	1HSL	Bahadur	1THE	Bahadur			2QB5	DCXtal
1B80	Bahadur	1I4G	Bahadur	1THT	Bahadur			2W20	DCXtal
1BC2	Bahadur	1IHB	Bahadur	1TOA	Bahadur			2X26	DCXtal
1BF6	Bahadur	1ILR	Bahadur	1TRN	Bahadur			2ZYZ	DCXtal
1BIN	Bahadur	1JFR	Bahadur	1URP	Bahadur			3C1D	DCXtal
1BKZ	Bahadur	1KPT	Bahadur	1VLZ	Bahadur			3H30	DCXtal
1BYO	Bahadur	1KWA	Bahadur	1XCA	Bahadur			3IRB	DCXtal
1C02	Bahadur	1MBL	Bahadur	1XGS	Bahadur			3ITA	DCXtal
1CFY	Bahadur	1ML1	Bahadur	256B	Bahadur			3LVD	DCXtal
1CKI	Bahadur	1MPG	Bahadur	2ATJ	Bahadur			3MG1	DCXtal
1CQX	Bahadur	1MSS	Bahadur	2BC2	Bahadur			3MHJ	DCXtal

D) Disordered proteins									
3KYS	1QZ7	2W2H	4E05	3FM7	1L0O	5BXV	1O6O	1DP5	3DBO
1KVD	3OUW	4V1T	2WJV	1S70	3V4Y	4BJT	4KYT	4X8K	4RWS
3FII	4J8R	4OWT	2FOO	1O9U	3DCG	3T0Y	1JPW	1T44	3MI9
3T5G	2O8G	4WXA	3T5V	2WSC	4XK8	1RH5	1HFE	2RF4	1UB4
3WYG	1AUI	2ZXE	4W4U	3U28	3H0G	1EE5	4IEA	5FCG	5DA7