

Supporting Information

ProBID-Net: A Deep Learning Model for Protein-Protein Binding

Interface Design

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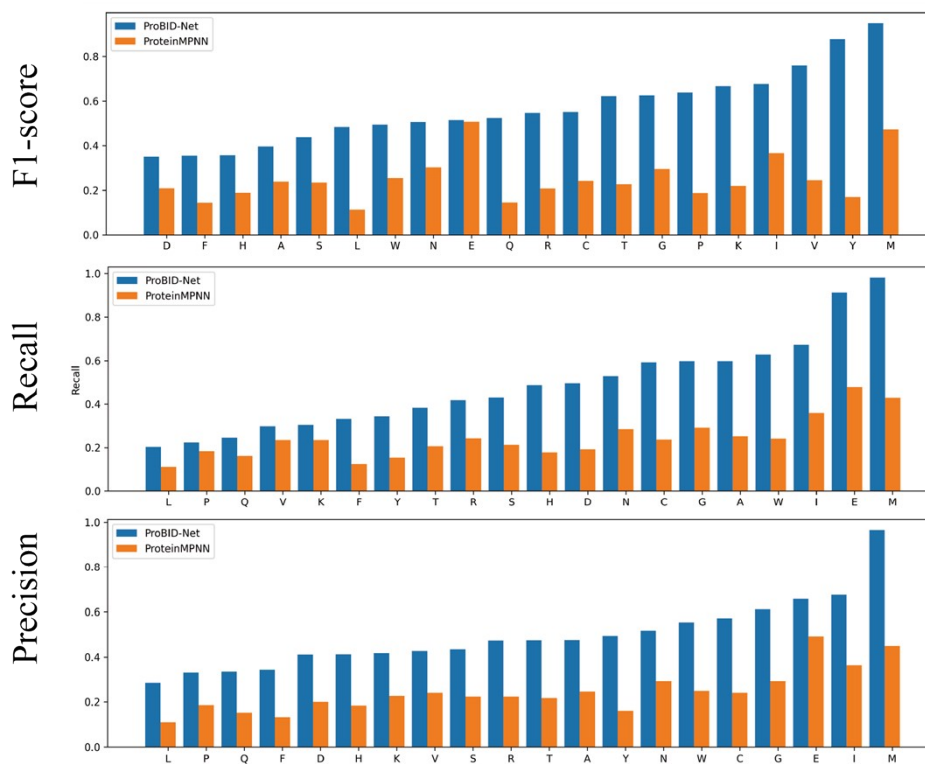
- Figure S1: Residue type Precision, Recall, F1_score
- Figure S2: Sensitivity of recovery to the initial placement of the ligand chain
- Figure S3: Correlation between protein-protein binding affinity and recovery rate
- Figure S4: Recovery on hotspot residue
- PDB IDs of test sets
 - Table S1: The number of docked structures at varying levels of structural deviation from the wild-type complex.
 - Table S2: TS920
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Residue type precision, Recall, F1_score

We further evaluated the accuracy of ProBID-Net in predicting specific amino acids and compared it to ProteinMPNN.

Precision represents the percentage of correct predictions out of all the predicted instances, recall indicates the percentage of wild-type amino acids that are correctly predicted out of all the actual instances, and the F1 score is a combined measure of precision and recall, providing a balanced evaluation of the model's performance. The results of our analysis show that ProBID-Net exhibits higher precision for most amino acids, especially for Met, Gln, and Tyr. Additionally, ProBID-Net demonstrates comparable recall and F1 scores to ProteinMPNN, indicating that it performs well in correctly identifying true positive instances and achieving a balance between precision and recall, shown in **Figure S1**. Furthermore, ProBID-Net shows a tendency to predict Met, Glu, and Ile with high accuracy. However, it is slightly less accurate than ProteinMPNN in predicting Phe and Leu. Despite this slight difference, ProBID-Net still performs well overall and proves to be a promising model for accurately predicting specific amino acids in protein sequences.

TS920



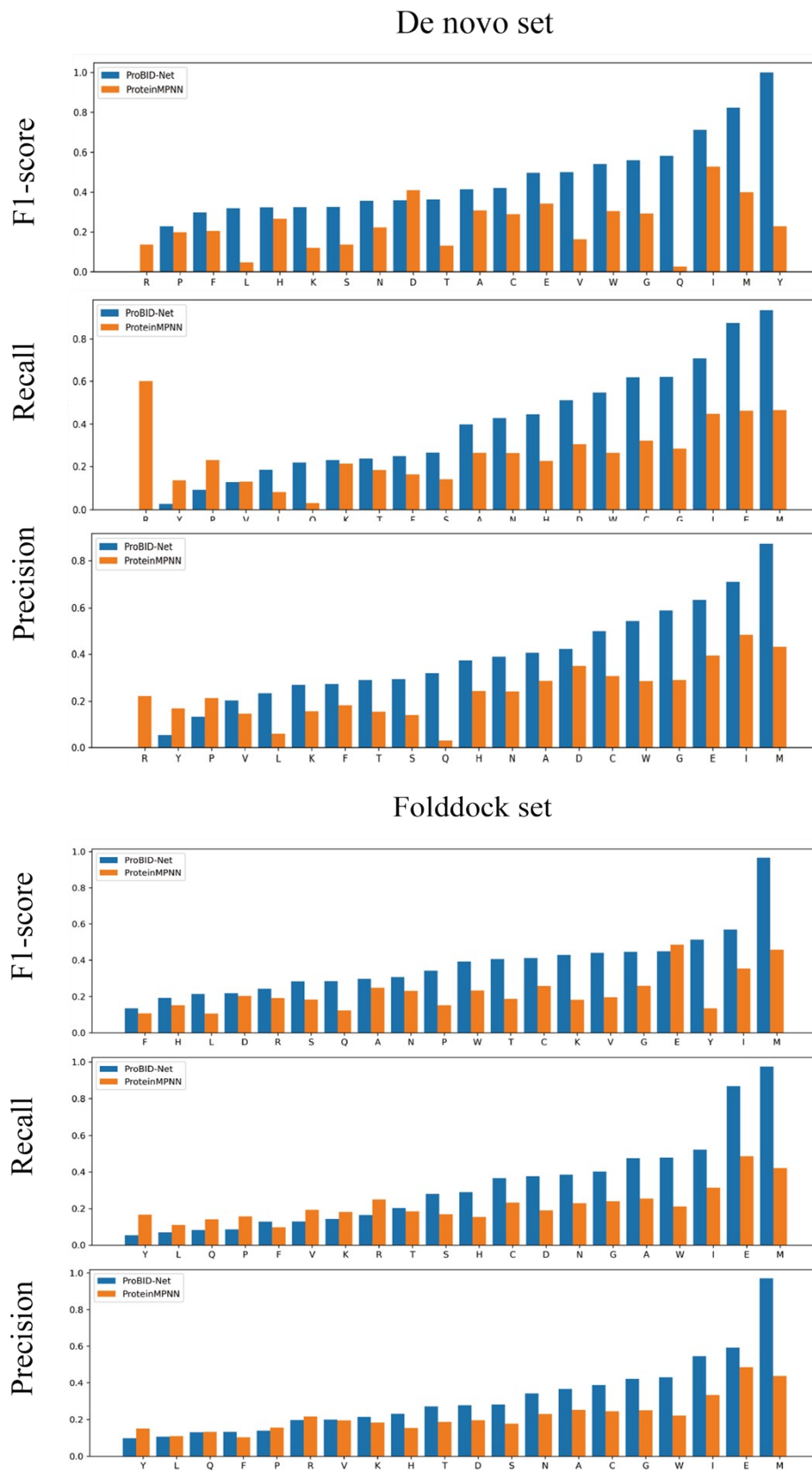


Figure S1. Recall, precision, and F1 score of ProBID-Net and ProteinMPNN for each amino acid on TS920, *De novo* set and Folddock set.

Table S1. The number of docked structures at varying levels of structural deviation from the wild-type complex.

Test Sets	RMSD < 1 Å Complex Count	1 Å < RMSD < 5 Å Complex Count	RMSD > 5 Å Complex Count	Wild-type Complex Count
denovo set	20	11	46	31
Folddock set	349	94	366	275
Ts920 set	175	59	157	141

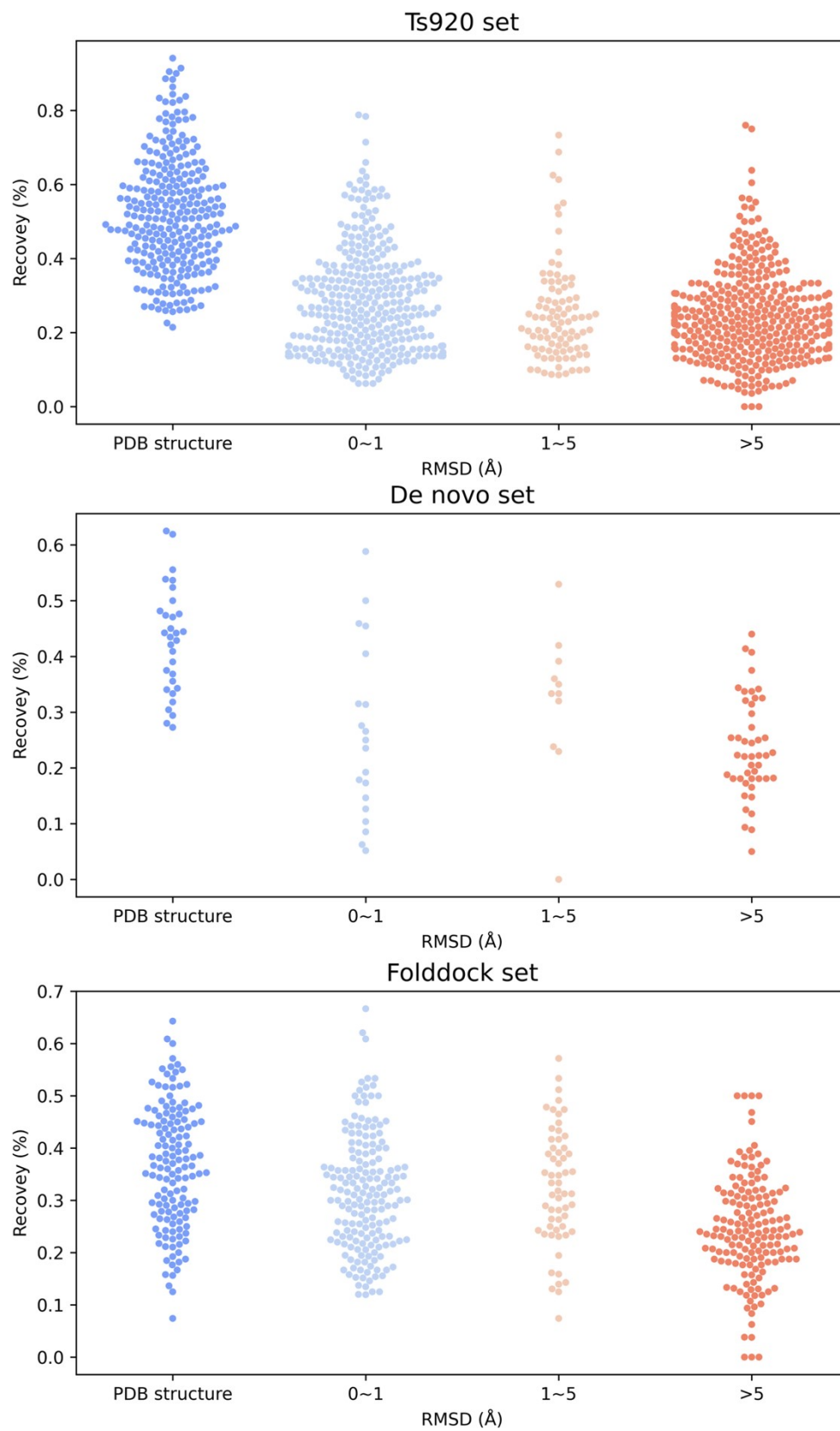


Figure S2. Distribution of predicted recovery in docked structures across the TS920, De novo, and Folddock sets, with different colors representing varying levels of structural deviations.

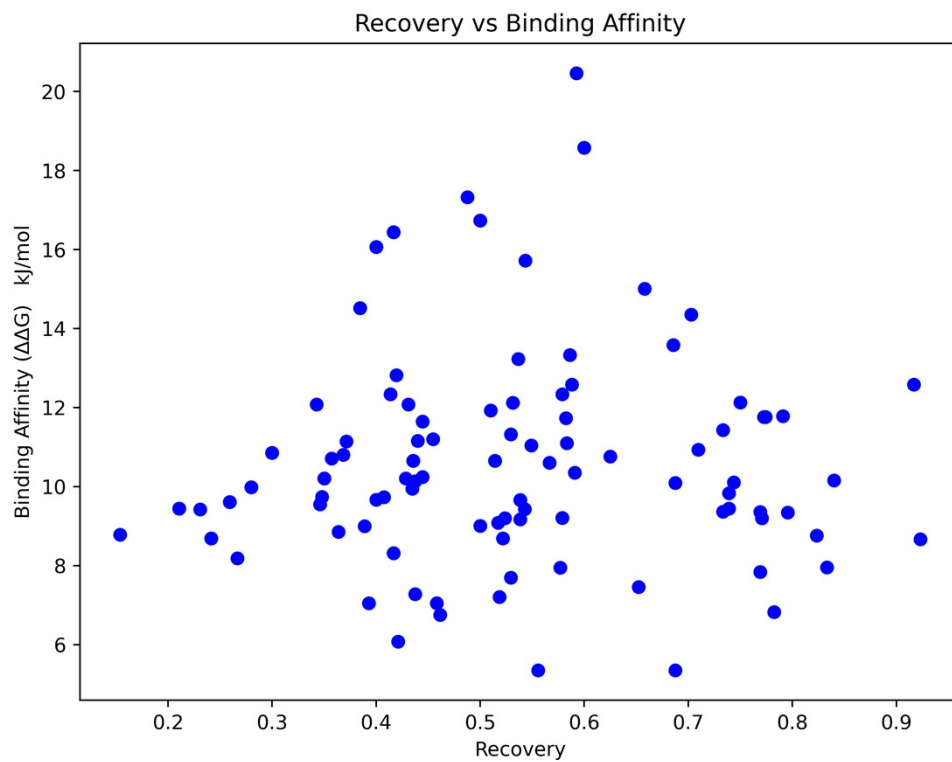


Figure S3. Recovery rate of ProBID-Net with respect to binding affinity of protein-protein complex.

Figure S4. Residue recovery of hotspots. Hotspot residues are represented by red crosses. Each protein-protein contact is represented by a blue dot.

PDB IDs of tested ligand pairs in each set

(1) TS920^{1,2}:

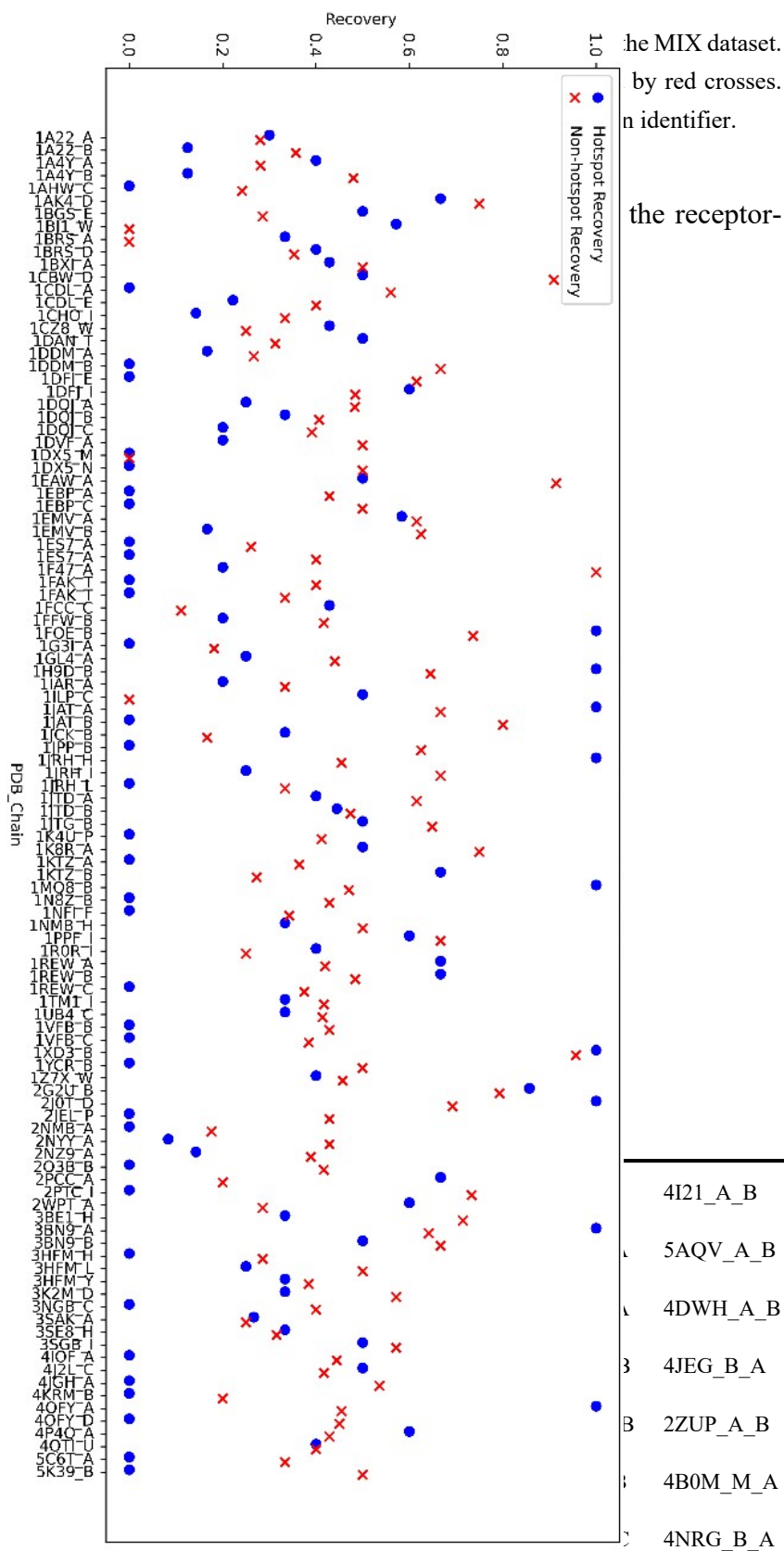


Table S2: The list of

4AG2_C_A	1Z0K_A					4I21_A_B
4ZPR_A_B	2D74_A					5AQV_A_B
1J2J_A_B	3IMQ_B					4DWH_A_B
3TUF_B_A	3ZJY_A					4JEG_B_A
3C5J_A_B	2VGO_A					2ZUP_A_B
3D65_I_E	4LLM_F					4B0M_M_A
4F0Z_A_B	1JCH_A					4NRG_B_A
1BXI_A_B	2P8Q_A_B	6SA7_A_B	6XUL_B_A	3CPJ_B_G	3UIR_A_B	1P9M_A_B
1ZBD_A_B	2QNA_A_B	4ONN_B_A	2P22_A_B	2G38_B_A	3X1L_B_A	3A8Y_A_B

3M7Q_B_A	3NVI_B_A	2Z6K_C_A	2DYM_A_B	3T62_B_A	2Y69_A_M	3TJ3_A_B
3D2E_B_A	2XAJ_B_A	3ZMS_B_A	4AFS_C_A	4LLD_B_A	4ZEQ_B_A	4OV6_G_A
1OL5_A_B	3HCU_B_A	7T2F_A_B	3NMU_B_C	1IXS_A_B	2C1T_A_B	4ZPH_A_B
4DJ9_A_B	5T5W_B_A	5WPL_A_B	1VG0_B_A	4F0Z_A_C	4KFZ_A_B	3KF9_A_B
2Y69_A_B	2Y69_A_D	3NMU_C_A	5T48_A_B	2GWW_A_B	4IF6_A_B	1R5I_A_B
3WOE_A_B	4KXQ_A_B	4ONM_B_A	3M3Z_A_B	4HLQ_B_A	2PMS_A_B	4QKO_A_B
4M6B_A_C	3TW8_B_A	3C5T_B_A	3L3T_E_A	3MZW_A_B	3W1Y_C_A	1J7D_B_A
2ZWE_A_B	3R2C_A_B	3ZMZ_B_A	4LN0_B_A	3KYS_A_B	1UJW_B_A	5EW5_E_A
4C0A_C_A	4ONL_B_A	3JZA_A_B	1DP5_A_B	1HR7_B_A	2X19_A_B	1RRP_A_B
3AWV_A_B	3RFZ_F_E	3SJA_A_B	4U8H_A_B	3IO8_A_B	2FYU_I_A	2BZW_A_B
3FZK_A_B	1T01_A_B	5HPS_A_B	3EFO_A_B	2XAS_B_A	3A36_A_B	2YPA_A_B
1HX1_A_B	6S9P_A_B	5H2W_C_A	2PQA_B_A	4H10_A_B	1T08_A_B	2HVY_D_A
1EGJ_L_A	6YWD_B_A	7AYE_B_A	4YL8_B_A	4UEM_A_B	5HPK_A_B	1QGK_A_B
3JZF_A_B	3O4O_B_A	1BH9_A_B	1RH5_A_B	4B8L_A_D	1B98_A_M	3DCG_B_A
6Q2X_L_A	4ZI2_A_B	4ROE_B_A	2Y69_N_Y	4ZP3_A_B	1WQ1_R_G	4W4L_B_A
5WPM_A_B	2HRK_B_A	2VOI_B_A	3DOE_A_B	2B5U_A_B	3KJL_B_A	1R6O_B_A
5D1L_A_B	4R6U_A_B	3W2V_B_A	4PBW_D_A	3ZN1_B_A	1WX2_A_B	3IDC_B_A
1NW9_A_B	3TDZ_B_A	3DOF_A_B	3Q9N_C_A	1VIW_A_B	3QC8_A_B	2QWP_A_B
5WLB_A_B	7NAM_B_A	3ZVQ_A_B	1PVH_A_B	3EJD_A_B	4S0H_B_A	3F62_B_A
3TNQ_A_B	2P22_A_D	1RE0_A_B	3X1L_B_C	6SA8_A_B	1IXR_B_A	1MG9_B_A
4K8R_C_A	3S90_A_B	4WBB_A_B	3TKL_A_B	3TZ1_A_B	1U35_C_A	3VHX_A_B
3N1G_A_B	1MBX_A_B	1BND_A_B	2QN6_A_B	4REQ_A_B	1I1R_A_B	1NH2_A_D
4ETW_C_A	3FZM_A_B	3QBT_C_A	4TKP_A_B	5C7J_A_B	3OG4_B_A	2QSF_X_A
3TJ5_A_B	1XWJ_A_B	4FMD_B_A	1MBV_A_B	1MIU_A_B	2EFH_B_A	7CEI_A_B
2ZWG_A_B	3VZA_A_B	5HPL_A_B	1ZW0_A_B	4BD9_B_A	4HPL_A_B	2CFH_A_B
2PMZ_G_T	4D18_E_H	6S8S_A_B	1Ytz_I_C	3O4O_A_B	4KB8_A_B	1N1J_A_B
3AX0_A_B	3D1M_A_B	3SL9_A_B	3M0D_D_A	3D5S_A_B	3E1Y_E_A	1B5F_B_A
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3AON_A_B	3SFV_A_B	1DHK_A_B	3IDB_B_A	4GOJ_A_B	3WHL_C_A	2V1D_B_A

1TY4_A_B	4U30_A_B	4D0G_A_C	2EQB_A_B	3H7W_B_A	4IZ7_A_B	3S48_B_A
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4ISL_A_B	4WWI_A_B	1X3W_B_A	2QWQ_A_B	2QVS_B_E	2YHO_B_A	3E20_A_B
2ERH_A_B	1C1Y_A_B	4C9R_C_A	2Y69_Y_N	4D18_M_N	7LF7_B_A	1TMQ_A_B
2D7C_A_B	3LAQ_B_A	4XT1_A_B	2OMX_A_B	4IAO_A_B	4C2V_A_B	1R6Q_A_B
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2WAX_A_B	3VZ9_B_D	4XT3_A_B	1MZ8_A_B	2XA0_A_B	3QHT_C_A	1O9K_A_B
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3V11_A_B	3HD7_F_A	4WLQ_A_B	1SQ2_L_N	3WO3_B_A	4IZA_A_B	1JAT_A_B
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1BUH_B_A	1A2X_A_B	2EFD_B_A	2OCF_D_A	2OMU_A_B	5ZAU_A_B	1ZR0_B_A
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3NMU_C_B	3FHI_B_A	4S0T_A_B	1A2X_B_A	1B8M_B_A	1BND_B_A	1BQL_Y_H
1BQL_Y_L	1BRC_E_I	1BVN_P_T	1BXI_B_A	1EMV_B_A	1F2S_B_A	1F45_B_A
1FR2_B_A	1GO3_E_F	1H9H_E_I	1IBR_B_A	1IRA_X_Y	1KI1_B_A	1M56_B_A
1MCV_I_A	1O5E_L_H	1O5F_L_H	1PPE_I_E	1QGE_D_E	1UKV_G_Y	2BCG_Y_G
2BTC_E_I	2F3C_E_I	2GYK_B_A	2GZE_B_A	2GZF_B_A	2GZG_B_A	2GZI_B_A
2GZJ_B_A	2PMZ_P_Q	2QSH_X_A	2STA_I_E	2STB_I_E	2VLN_B_A	2VLO_B_A
2VLP_B_A	2VLQ_B_A	2WPT_B_A	3BT1_B_A	3CF6_R_E	3D3B_J_A	3HO5_H_B
3IFQ_C_A	3MZW_B_A	3NC1_A_C	3P71_T_C	3QWQ_B_A	3REA_B_A	3RLF_A_B

3UYO_D_A	3VZ9_B_D	3VZA_C_A	3WO4_B_A	4AG1_C_A	4CIN_B_A	4D8D_B_A
4EMZ_E_A	4FMD_F_A	4HRL_A_C	4K5A_B_A	4K5B_C_A	4K8R_L_H	4MGI_E_R
4MGK_R_E	4MGY_R_E	4MGZ_R_E	4N9G_B_A	4Q5U_C_A	4QVE_B_A	4R6U_B_A
4RIW_B_A	4RIY_B_A	4U32_A_X	4U6Y_B_A	4URU_R_S	4URV_R_S	4URW_R_S
4URX_R_S	4URY_R_S	4URZ_R_S	4US0_R_S	4US1_R_S	4US2_R_S	4Y99_C_B
4YII_A_U	4YIR_X_A	4YQX_L_A	5DLQ_B_A	5FUG_K_J	5Z2Q_B_A	6ER6_B_A
6ERE_A_B	6O9I_E_D	6P4A_L_H	6P4B_C_A	6P4C_L_H	6XTG_L_H	6XUD_L_H
6XUK_L_H	7B4T_A_B	7R9D_L_H	7URX_L_H			

(2) Folddock set^{3,4}:

Table S3: The list of protein-protein complexes in Folddock set

3G5O_C_D	3EGW_B_C	4P78_A_D	5N9J_E_C	3NCE_A_B	3MHS_A_E	4WEM_A_B
2FM8_A_C	2PF4_H_D	1OQE_I_Q	3TUI_C_A	3LVK_A_B	4FOU_A_C	1OFH_A_G
5LDD_C_B	5T59_A_B	1H3O_A_B	3C0T_A_B	7EIV_A_C	1N6J_G_A	2Y69_N_S
3HTK_B_C	4Z96_C_A	5T59_A_C	5J1S_A_B	2Y69_N_P	2F8X_C_K	1IAR_A_B
5T5I_B_A	4U7U_A_K	4CMM_A_B	3H0G_N_U	5MB9_A_D	4A8X_A_C	1I7Q_D_C
1WVE_A_C	2WP0_B_D	3HRD_A_D	4OO1_H_J	5LSJ_C_Q	4WJ3_H_I	5AWF_B_D
2FTK_A_E	3GQI_B_A	2CLY_B_C	3RNQ_A_B	4GAM_I_M	4WQO_D_A	3R84_U_V
5LG4_A_B	5VOB_A_B	1NH2_A_D	2R6A_C_B	3D6N_B_A	1KF6_N_M	4DAY_C_A
4UB8_A_I	4Z2M_B_I	3U6X_Y_D	5L6W_C_L	1CI6_B_A	3T5V_C_B	3JQO_I_k
1J34_A_C	2NS1_B_A	2Y69_P_N	4RT6_B_A	3EUH_A_C	2G48_B_D	5LDD_B_A
2I2X_I_J	1IS8_H_S	1ES7_A_B	2J56_H_A	2PMZ_Q_W	2WDQ_B_C	5DMV_D_C
4UI1_A_D	4NWP_E_C	5T5I_D_B	2Y69_B_E	4UFR_A_B	4FAO_M_Q	4KT5_A_C
4DI3_C_E	4Q2U_B_A	2Y69_B_I	5HY3_A_B	4J7C_B_K	5IBW_C_A	5FU7_E_G
3CF4_A_G	5IUK_E_F	3KFU_I_B	3MHS_E_B	4JLQ_A_B	4RS1_A_B	3TND_B_A
3VYT_A_B	4UB8_B_L	5UFU_B_A	4FXE_B_E	3NFG_D_C	4H44_B_C	3KXE_C_A
5B2G_D_C	3GZ2_P_B	2F4M_B_A	3MHS_A_D	5F5T_C_A	4EOZ_C_D	5AWF_D_B
5B0O_G_C	3N9N_C_A	5ABV_F_E	4DJD_F_B	1JR3_E_B	3D6N_A_B	4FQ3_A_B
1PB_Y_C_A	5N9J_U_Z	5WXM_B_V	2Y69_Y_N	3JQO_k_l	5UFU_A_B	3VYT_B_C
4Z2M_B_G	3T97_C_B	1YAR_C_S	2AW2_A_B	2FYU_A_K	5L9W_A_C	2FYU_A_G
5J9T_F_H	5V6T_A_B	4JLQ_B_A	1JB0_C_A	1NH2_A_B	2Y69_E_I	2Y69_O_U
4A8X_B_A	5IM5_A_N	4D18_B_F	1G1X_C_A	4DX8_B_H	4M70_I_J	2F9I_B_A
4OWT_A_C	5LSK_P_N	4F0Z_C_B	2CLY_D_E	2Y69_A_M	1BOU_B_A	5DOQ_B_A

5I9E_A_E	3KFU_B_I	1H59_A_B	1UB4_A_C	3O4O_A_B	4B7Y_C_A	5T5I_F_B
2ZP8_B_G	1M56_I_B	5LSB_A_B	4UB8_Y_Z	1EEX_L_M	2CZV_A_C	1ZAV_A_V
2QFA_A_B	3L75_R_T	3RZO_C_J	5N9J_W_U	5J1S_B_A	5FVD_A_B	4AQR_A_D
2XPI_B_A	3KZ4_H_B	1IKN_A_D	5BNX_C_B	3TJZ_B_A	5CCB_A_B	3U6X_D_Y
1L1O_D_A	2FYU_C_E	5N9J_A_D	4B8C_H_C	4A8J_E_D	4Z80_C_A	3U88_C_M
4H44_A_D	5N9J_G_B	4FAO_d_b	4ODB_E_B	4BV4_M_R	4H44_A_B	4CCN_D_B
1ORY_B_A	4Z6Y_A_D	5WGB_B_A	5IMT_A_D	1GO4_F_B	5F5T_A_C	5T59_C_A
5LSJ_G_E	2ZZD_L_J	3W15_A_C	3M9S_F_3	2IVF_C_B	2J56_H_L	3F3F_D_B
5O7X_I_G	1SXJ_G_B	2VPZ_G_F	3TVT_A_B	2FYU_I_A	5MSM_A_B	4DAY_A_C
2AQ2_A_B	3A5Z_C_D	4JCV_C_E	3X1L_G_D	4NWO_A_B	4U4C_A_B	4WWX_E_Y
1PRT_K_G	2QFA_B_C	4CFR_B_Q	1NBW_A_B	2FYU_A_I	5N9J_W_S	3MHS_C_A
5LDA_A_B	1GNG_A_X	1NH2_A_C	7K01_1_6	5LSJ_C_G	1YAR_S_C	2Y69_S_P
5AAW_Y_G	1Q90_D_C	4UB8_E_R	4D18_A_F	4I9X_C_B	5LDD_C_A	4Z2M_H_B
5VJI_D_F	5NT7_C_D	4OJK_C_A	5J9T_B_C	5N9J_B_C	2PT7_D_H	2ARP_A_F
3WWN_A_B	3VIQ_A_B	4JHJ_C_A	4LNU_A_K	4ZRP_C_A	5JA4_B_D	5HXG_D_C
5K23_A_C	5AAW_Y_E	5DMV_C_D	5E8J_B_D	1PRT_E_F	4UQI_A_M	4XWJ_A_B
3TJZ_C_B	1UF2_K_A	5LTW_F_G	1HBX_G_B	5HK5_E_A	3IAX_B_A	5JPO_E_A
2Y69_P_S	4HI0_A_B	3N9U_B_C	1XDT_R_T	1PXV_B_D	1XOU_A_B	7M5F_B_A
5BWA_B_A	2PMZ_B_P	2PMZ_K_C	3S8G_A_C	5FIR_D_C	3KFU_H_I	4JIN_F_L
2B4J_A_D	5T89_V_X	3RZO_B_K	4ZRK_G_C	5GQQ_B_D	4H44_C_E	5LSJ_D_B
2Z5K_B_A	3MK7_D_E	2Q86_C_D	4D18_I_J	2Y69_G_C	4HSA_F_E	5F5P_E_G
5O7X_G_H	4XGC_C_F	1B33_N_E	1XDT_T_R	2VPZ_A_B	4H44_B_G	2J56_L_H
3TND_A_B	1XF6_A_C	5T5I_A_B	4H44_A_G	3WWN_B_A	4IFD_C_J	4IFD_C_I
4WNL_E_D	1QS0_B_A	3T12_C_A	3VA2_C_A	3VU9_A_B	3UTM_C_B	2FYU_G_D
5K04_A_B	4XGC_F_C	5LSK_N_P	3TUJ_A_C	3TJZ_A_B	3A0R_A_B	5T5I_K_J
3M4W_A_E	1GL2_A_D	2XKO_C_B	3NMU_C_A	1JB0_D_L	1YFN_A_E	5ET0_D_C
5HY3_B_A	3FBI_A_B	5LXT_A_F	2PMZ_H_A	2ZXX_F_E	5FFO_A_G	4M5D_A_B
4F0Z_A_B	3X1L_A_F	1OR7_B_F	5BNX_A_D	4OO1_C_J	4U7U_U_P	2JF1_A_T
5IIB_A_B	5N9J_A_B	2IVF_A_B	5IFG_A_B	5B2G_F_A	3RZO_C_L	2F8X_K_C
1Q90_A_R	2BA1_E_B	3PXG_f_F	3ULY_B_A	4CO6_C_E	5O7X_E_F	2PU9_A_B
6VN1_A_H	3UTM_B_C	5I2D_F_G	3KFD_J_A	4QPG_C_A	3R45_A_C	3PNL_A_B
3TNU_A_B	3K51_B_A	4IIT_A_B	2FYU_C_G	3KXE_A_C	4YYP_A_B	3VEP_C_A
4HFK_A_B	4U7U_M_V	3BPO_C_B	5X1E_A_C	3AYH_B_A	1GXD_A_C	1PRT_D_B
4ZRI_C_A	4LD3_B_A	5I2D_A_H	5N9J_B_G	4E6K_D_H	4XGC_C_E	1LRW_B_A
5FU7_B_A	3BK3_C_A	5V3N_A_B	3R84_V_U	5N9J_D_G	4H44_G_B	1IK9_A_C
1EXB_A_E	2Y69_C_G	3U60_G_C	5NLB_B_A	2QOO_A_C	5UA4_A_B	3CL3_A_D
3TVT_B_A	5E8J_D_B	5BS7_C_E	5WXM_V_B	2HTM_G_C	3BRV_B_C	4PUF_B_D
5ABV_E_F	4EBA_H_C	5WYL_C_D	3NFG_C_D	2P22_A_C	5FM5_M_P	5IUK_F_E

4H44_B_A	4GAM_C_B	1YA5_B_T	5FFO_B_D	4D18_F_A	3KFD_G_K	4UB8_A_B
2NQ2_A_C	4UB8_I_A	1WVE_C_A	2BQ1_E_I	3IKO_H_I	4UQI_B_S	1PRT_F_E
5N6Y_A_C	2F8X_C_M	1KF6_B_D	1YKH_A_B	2Y69_D_E	4UB8_T_A	4UB8_K_Y
5JAA_D_A	5T70_A_G	4XIZ_A_N	2QFA_B_A	1H2S_A_B	4HZU_S_T	5N9J_R_G
4UB8_A_O	5F5S_A_B	2Y69_A_B	4U65_A_E	3OIQ_A_B	5IM5_N_A	4OMF_A_G
3BES_R_L	4XPM_C_A	5KTB_B_C	5T5I_J_K	5FFO_G_A	5T5W_B_C	1GL2_A_B
4CYM_A_D	4G2V_A_B	4A8X_A_B	5BQC_A_B	4U7U_W_V	1EEX_M_L	4XB6_H_G
5TCS_C_A	3NMU_F_A	4DL0_G_E	5H2F_F_J	2FYU_J_K	4XGC_C_B	4FAO_Q_M
1YKH_B_A	3SJL_B_E	2ZME_B_D	4H63_R_V	2P22_A_D	4OWT_A_B	1N6J_A_G
3X1L_A_C	1JB0_D_C	3NMZ_A_C	5T5I_B_G	5O32_J_F	3H0G_L_B	2ZXX_E_F
3BG1_A_B	5FU7_G_E	2DOQ_B_D	5VOB_B_D	2NPS_D_A	1KKM_A_I	5B58_T_B
7QIH_A_D	2P58_C_A	3HUG_I_J	4NTW_B_A	3DIN_C_A	5FIR_C_D	1UW4_D_C
4CYM_D_A	4KP3_A_C	5BNX_B_C	5FM5_P_M	5L6W_L_C	3VA2_A_C	5N9J_B_E
1JB0_F_J	3T5V_B_C	3INB_A_D	2NN6_I_F	4DCK_A_C	3U60_C_G	2D1P_D_F
5JHF_E_F	5N9J_A_R	1W85_I_B	1J34_C_A	4DXR_A_B	2IZV_A_C	4UB8_A_T
3ISM_C_A	1GHQ_A_B	1JB0_A_D	4XWJ_B_A	5LOP_A_C	1L1O_B_C	2ARP_F_A
5EKQ_A_E	5O7X_F_E	1P9M_B_C	2FMM_C_E	5F74_B_A	2PT7_H_D	4PKF_A_C
3FWB_A_B	2IJ0_B_C	4XHJ_B_A	4GAM_B_C	5MU7_A_B	3TIX_A_B	5N9J_A_E
2PMZ_B_N	4XPM_A_B	4P1B_A_I	1TTW_A_B	3LCB_B_C	4N3Y_A_C	1QS0_A_B
2Y69_U_O	4IIT_B_A	4D18_E_H	4OWR_A_C	4DL0_C_G	5N9J_G_E	3RLF_E_G
7EL1_A_E	3EAB_G_A	2WJV_B_E	4UB8_B_H	3GZ2_B_P	5LSJ_A_D	2CLY_C_A
3M4W_E_A	1CCW_D_C	4ZHY_B_A	3C0T_B_A	5JW7_A_B	1LTS_C_E	5LSI_D_E
7QIH_A_B	3HRD_H_F	4YMU_C_J	4ME7_C_F	3X1L_B_C	3GQI_A_B	4MCT_A_B
4JMF_B_A	1EEX_L_E	2V53_A_D	1SR4_B_A	1TH8_A_B	3U52_E_A	3U7U_D_J
5X1E_C_A	5F0J_B_A	3QKS_A_C	3RFZ_E_F	1KF6_N_O	3VEP_A_C	3N9U_C_B
2NV2_K_L	4G4S_O_P	5N9J_B_A	2IZV_C_A	2Y69_A_T	5T89_X_V	1NH2_D_C
4XGC_A_D	4B8C_C_H	4JMF_A_B	5JWO_B_A	2VPZ_F_G	4U4C_B_A	3L75_S_Q
2OZ4_H_A	5DLQ_B_C	1KF6_D_C	4YMU_J_C	5F0J_B_C	7NJ0_A_C	3OIQ_B_A
3DIN_A_C	5MSM_B_C	3M9S_3_F	3N9N_A_C	3D31_C_A	2FYU_D_H	2NPS_C_D
3DBO_B_A	4D18_M_J	4H63_V_R	5N9J_U_W	1G1X_A_C	2FYU_K_A	2AZE_C_B
4UB8_U_B	4H9N_A_C	2PQN_B_A	4KT5_C_A	1XOU_B_A	4D18_M_N	2RDD_B_A
4GF3_A_B	2ZZD_J_L	3RFZ_F_E	4NRH_A_D	5JA4_D_B	5N9J_A_W	1LRW_A_B
2BQ1_I_E	1UF2_A_K	3O6Q_D_A	4QLP_B_A	5KBX_A_B	4DL0_E_I	5F4E_B_A
4X8K_A_B	2IZO_A_C	3PNL_B_A	4XGC_A_B	4XGC_B_E	5T5I_B_F	5I2D_G_F
2A6Q_C_F	5HU3_B_A	1XKP_A_C	3H0G_B_J	5KWY_C_B	2PMZ_H_K	4B7Y_A_C
4I98_A_C	5DA9_A_C	2BRQ_A_C	5DLQ_B_F	4WJ3_A_P	4KP3_B_F	2RDD_A_B
2QFA_C_A	3BOW_B_C	1JB0_A_F	3AYH_A_B	2XZE_A_Q	2FYU_A_C	1JNR_A_B
2PMZ_K_H	2WIU_C_D	3KFU_H_J	4DCK_C_A	3D31_A_C	4IN3_D_C	4LD3_A_B

1JB0_A_E	2XKO_B_C	4UB8_A_V	3P8C_B_F	2CLY_A_C	2J12_B_A	3KP1_E_A
4IFD_I_C	2WJN_L_H	5B5W_A_U	5TDY_C_D	3KFD_B_F	4JOI_B_C	3MHS_A_B
4NRH_D_A	2WJV_E_B	5EOF_B_C	3DIN_A_E	2P22_A_B	5NVL_D_C	2PMZ_E_K
4H44_F_G	3M91_A_B	3OC3_C_A	4BSZ_A_B	117Q_C_D	7LDG_A_B	5T5W_C_A
5F1B_C_A	2J56_A_H	2V5P_B_C	2WJN_L_C	3PHF_3_4	3W15_C_A	5DMB_A_D
3L75_E_J	6R17_B_A	1W85_C_D	3A5Z_D_C	5O7X_H_G	5CGQ_B_A	3N3A_B_C
4LL1_A_B	3H0G_B_L	3A0R_B_A	3U52_A_E	4CRY_B_G	3O4O_B_A	1GHQ_B_A
3MHS_B_E	2Y69_X_Q	1TII_C_E	4RT6_A_B	3MMY_C_D	5F0J_C_A	2J56_L_A
5IXI_B_A	5UK4_n_N	2P58_A_B	2PMZ_P_B	3S8G_A_B	5B64_A_B	5D6H_A_B
4CRY_G_B	5LGD_A_B	4H44_G_A	3ALZ_A_B	3RZO_C_K	11S8_S_H	2PMZ_C_K
4QAF_A_D	3NMU_C_B	5GK9_A_B	3S8G_C_B	4BFI_A_B	4WJ3_K_M	4WZA_D_H
5H2F_J_F	5JW9_A_B	5T59_E_F	3HRD_H_G	2NV2_L_K	1L0O_B_C	6VN1_B_A
5VXZ_B_D	5O7X_G_I	4JHJ_A_C	4JJN_E_L	5LXT_A_E	1ORY_A_B	1XU2_R_A
2YFV_A_C	2P58_A_C	2R6A_B_C	5N9J_C_A	4HKJ_N_P	2AS5_F_N	2PMZ_A_H
4XGA_A_B	2PF4_D_H	3AB0_E_D	1KKM_I_A	4PBY_B_D	4TQU_M_Q	5KBX_B_A
6R17_A_C	7QIH_B_A	2Y69_D_A	2Y69_L_M	7LDG_B_A	4FAO_d_W	2EQ7_B_C
4B8C_A_D	3HHZ_A_K	1GVN_C_D	5G1X_A_B	5LB7_A_B	1GO4_B_F	3N3A_C_B
2BA1_B_E	1SR4_A_B	2F4M_A_B	5JFZ_E_F	4XGC_D_A	5LDD_B_C	2P5T_E_F
2FYU_F_C	1JB0_D_A	4F0Z_A_C	3GE3_A_C	4AJ5_I_S	5IXI_A_B	5FU7_A_B
3EAB_A_G	5N9J_B_D	4ODB_B_E	2Q7N_A_B	5GJK_A_B	5N9J_A_G	3P8C_D_F
4NTW_A_C	4B8C_D_H	5M72_A_B	4UB8_Y_K	1P9M_A_B	7QIH_D_A	3CR3_B_D
3RFZ_D_E	4HI0_E_A	4ZRK_C_G	1FYH_A_B	3X1L_B_A	3PIN_B_A	1PRT_B_F
5EP6_A_B	2PU9_A_C	5N9J_Z_S	4DJD_E_B	2AVU_E_B	1SXJ_B_G	4OMF_B_A
2PMZ_G_T	4W4O_A_C	4XGC_E_C	1U2G_B_C	4ZK7_W_E	4EBA_C_H	5CGQ_A_B
2Y69_I_E	4XPM_C_B	1PRT_G_K	5DLQ_F_B	5FU7_A_D	4IFD_A_G	5T5W_B_A
3L75_D_E	4KP3_F_B	3L2O_B_A	3KFD_F_B	3MK7_E_F	5F0J_A_C	5FVD_B_A
5EP6_B_A	3L75_E_D	4Q2U_A_B	1JB0_L_D	1JR3_B_E	5FFO_D_B	5N9J_S_U
5LGD_B_A	3MZK_C_D	2F8X_K_M	5BNX_B_D	5JPO_A_E	5UA4_B_A	4XGC_A_E
1OR7_F_B	3S JL_B_F	4HX3_G_H	4XXB_A_B	5BWA_A_B	2WJN_H_L	1TAF_B_A
3L82_A_B	3NMU_B_C	5N9J_A_S	2W19_B_D	5NLB_A_B	5NT7_D_C	5CX3_A_E
3V5W_A_B	2Y0N_A_E	5CSF_C_B	3RKO_E_F	3KFU_I_H	3ZDL_B_A	5UNI_B_A
4UB8_u_o	2PMZ_A_L	4WPX_A_B	4LL8_E_A	1TH8_B_A	7UUS_I_J	5T5I_C_A
4U7U_B_E	3O4O_B_C	3Q33_A_B	1XRS_A_B	2PU9_B_A	2W19_D_B	4XB6_B_D
4NTW_A_B	5FQ8_B_G	1FM0_D_E	3LCB_C_B	4UB8_j_e	2Y69_A_D	5GJK_B_A
5N9J_E_G	5LSJ_B_D	1ZT2_B_A	7UBZ_A_B	4J7C_K_B	5WUR_A_C	2Y69_N_Y
2P58_B_C	2ZXE_A_G	4UB8_U_V	4QPG_A_C	2PU9_C_A	2Q0O_C_A	7EIV_C_A
2WDQ_E_F	2WDQ_F_E	2FYU_C_D	5BNX_A_C	5N6Y_C_A	5T59_B_A	2PMZ_V_G
5KL1_A_B	4ZRP_A_C	6TMM_A_B	3BK3_A_C	2PMZ_G_V	3MHS_B_C	2Y69_S_N

4ZRI_A_C	5KL1_B_A	4H9N_B_C	4NQW_B_A	2GH0_C_A	4JN_L_E	4UB8_B_O
5N9J_G_S	3EGW_C_B	3RZO_J_C	3RZO_K_C	3BRV_C_B	5LPU_D_B	1P9M_A_C
1M56_D_C	2WDQ_C_B	4Z80_A_C	3NCE_B_A	4IFD_G_I	4L63_A_C	3TQ7_Q_A
4ZHY_A_B	5LXR_B_A	4IFD_I_K	2PJW_H_V	4UB8_m_l	2PQN_A_B	4E6K_H_D
4FAO_b_d	4GAM_L_I	5T5W_A_C	1B33_E_N	4FBW_A_C	3EUJ_A_B	3O4O_A_C
3IJ2_B_X	4WPX_B_A	5FQ8_D_E	1FXK_A_C	3RLF_F_E	4XB6_E_G	5NXB_B_C
2P5T_F_E	3X1L_D_G	2AS5_N_F	2QIY_A_C	2QFA_C_B	1JB0_C_D	5J9T_C_D
3WWT_A_B	1T0F_A_C	1BOU_A_B	1FYH_B_A	1H2S_B_A	1H59_B_A	1IAR_B_A
1JNR_B_A	1M56_B_A	1NBW_B_A	1M56_C_A	1P9M_C_A	1OFH_G_D	1U2G_C_A
1PB_Y_A_B	1TAF_A_B	1TTW_B_A	1W85_B_A	1XRS_B_A	1ZT2_A_B	2AQ2_B_A
2AVU_B_A	2AW2_B_A	2F9I_A_B	2GH0_A_B	2IVF_B_A	2NS1_A_B	2Q7N_B_A
2VPZ_B_A	2ZXE_B_A	3BG1_B_A	3BPO_B_A	3DBO_A_B	3F3F_B_A	3FBI_B_A
3ISM_A_B	3K51_A_B	3KFD_A_B	3LVK_B_A	3NMU_A_B	3OC3_A_B	3PIN_A_B
3Q33_B_A	3RLF_A_B	3RNQ_B_A	3S8G_B_A	3T12_A_B	3T97_B_A	3TNU_B_A
3ULY_A_B	3V5W_B_A	3VU9_B_A	3WWT_B_A	3ZDL_A_B	4BFI_B_A	4BSZ_B_A
4CMM_B_A	4DJD_B_A	4F0Z_B_A	4FQ3_B_A	4G2V_B_A	4GF3_B_A	4HFK_B_A
4HI0_B_A	4I9X_B_A	4LL1_B_A	4M5D_B_A	4MCT_B_A	4NQW_A_B	4NWO_B_A
4OJK_A_B	4OWT_B_A	4RS1_B_A	4UFR_B_A	4XGA_B_A	4XHJ_A_B	4XPM_B_A
5B58_B_A	5BQC_B_A	5CCB_B_A	5D6H_B_A	5MSM_B_A	5DOQ_A_B	5F1B_A_B
5F4E_A_B	5HK5_A_B	5IBW_A_B	5IFG_B_A	5JAA_A_B	5K04_B_A	5LDA_B_A
5LG4_B_A	5LPU_B_A	5MU7_B_A	5UNI_A_B	5WGB_A_B	6TMM_B_A	7M5F_A_B
7UBZ_B_A	7K01_6_4	7UUS_J_I				

(3) De novo set⁵⁻¹⁹:

Below is the De novo set list. Each row represents the PDB ID of a ligand-receptor complex, allowed by the count of correct residues, the count of interface residues, and the recovery of interface residues.

Table S4 The list of protein-protein complexes in De novo set

PDB ID_ligand_receptor	Count of correct residues	Count of interface residues	Recovery of interface residues
3LHP_T_IM	2	19	0.11
3R2X_C_AB	5	18	0.28
3ZUV_B_A	8	19	0.42
4GLA_D_A	11	19	0.58
4GLV_B_D	8	18	0.44

4GN3_B_A	7	16	0.44
4GN4_B_A	10	18	0.56
4JW2_A_B	8	20	0.4
4JW2_B_A	7	18	0.39
4JW3_C_A	10	22	0.45
4N9G_C_AB	8	17	0.47
5OOV_A_B	16	27	0.59
6BZX_A_B	19	44	0.43
6DKM_A_B	15	41	0.37
6DKM_B_A	9	36	0.25
6DLC_B_A	12	25	0.48
6DLM_A_B	18	38	0.47
6DLM_B_A	6	35	0.17
6DM9_A_B	23	42	0.55
6DM9_B_A	18	43	0.42
6DMA_A_B	12	34	0.35
6DMA_B_A	14	35	0.4
6DMP_A_B	18	47	0.38
6DMP_B_A	19	52	0.37
6F0F_B_A	12	21	0.57
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6F0G_C_A	10	19	0.53
6G4J_B_A	15	27	0.56
6GB1_B_A	5	18	0.28
6MBB_B_A	12	17	0.71
6MOK_A_B	7	29	0.24
6MOL_A_B	8	22	0.36
6NDZ_B_A	17	41	0.41
6NE1_B_A	22	35	0.63
6NE2_B_A	15	32	0.47
6VFH_A_B	4	13	0.31
6VFH_B_A	4	17	0.24
6VFI_A_B	10	23	0.43
6VFI_B_A	12	16	0.75
6VFJ_A_B	4	14	0.29
6VFJ_B_A	4	11	0.36
6WMK_A_B	8	21	0.38
6WMK_B_A	6	21	0.29
6WRW_C_A	12	23	0.52

7A48_B_A	4	15	0.27
7A4D_E_A	18	37	0.49
7A4T_B_A	16	18	0.89
7A50_B_A	22	32	0.69
7F69_C_A	7	13	0.54
7JZM_A_B	7	17	0.41
7JZU_A_B	6	20	0.3
7L5M_B_A	23	45	0.51
7MWQ_D_C	10	24	0.42
7MWR_A_B	7	17	0.41
7UHB_K_C	9	23	0.39
7VG7_B_A	2	21	0.1
7XFR_B_A	5	13	0.38
7XYQ_B_A	8	21	0.38
7ZSD_P_M	7	21	0.33
8AW4_A_B	12	26	0.46
8AW4_B_A	15	27	0.56
8DCE_H_A	10	23	0.43
8DVN_B_A	9	14	0.64

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