

Supplementary Materials

Tables S1 and S2

Table S1. The 6,497 protein-peptide complex crystal structure records meeting the filtering criteria were retrieved from the PDB database

The filtering criteria:

- (i) Macromolecule types: only protein entities, no nucleic acids;
- (ii) Experimental method: X-ray diffraction;
- (iii) X-ray resolution: $\leq 3 \text{ \AA}$;
- (iv) Number of chains in biological assembly: ≥ 2 ;
- (v) Length of at least one chain: 5–30;
- (vi) Sequence identity: $\leq 30\%$.

The PDB records:

148L, 1A07, 1A08, 1A09, 1A0M, 1A1A, 1A1B, 1A1C, 1A1E, 1A1M, 1A1N, 1A1O, 1A2C, 1A30, 1A3B, 1A3E, 1A3R, 1A46, 1A4W, 1A5G, 1A5H, 1A61, 1A6A, 1A7C, 1A81, 1A9E, 1AA5, 1AB9, 1ABI, 1ABO, 1AD8, 1AE8, 1AFE, 1AFQ, 1AGB, 1AGC, 1AGD, 1AGE, 1AGF, 1AHT, 1A18, 1AIX, 1AKJ, 1AL2, 1AL4, 1ALX, 1ALZ, 1AMT, 1AO7, 1APT, 1APU, 1APV, 1APW, 1AQ7, 1AQC, 1AQD, 1AR6, 1AR7, 1AR8, 1AR9, 1ASJ, 1ATI, 1AV2, 1AVF, 1AVP, 1AWF, 1AWI, 1AWQ, 1AWR, 1AWS, 1AWT, 1AWU, 1AWV, 1AXD, 1AY6, 1AYA, 1AYB, 1AYC, 1B05, 1B07, 1B0G, 1B0H, 1B0R, 1B1H, 1B2H, 1B32, 1B3F, 1B3G, 1B3H, 1B3L, 1B40, 1B46, 1B4H, 1B4Z, 1B51, 1B52, 1B58, 1B5G, 1B5H, 1B5I, 1B5J, 1B6H, 1B6J, 1B7H, 1B7X, 1B8H, 1B9J, 1BA8, 1BB0, 1BBR, 1BBZ, 1BC5, 1BCK, 1BCU, 1BD2, 1BDW, 1BE9, 1BHF, 1BHX, 1BII, 1BJR, 1BK6, 1BKV, 1BM2, 1BMB, 1BMM, 1BMN, 1BQH, 1BR8, 1BS6, 1BS8, 1BT6, 1BW8, 1BX2, 1BX9, 1BXX, 1BY5, 1BYZ, 1BZ9, 1BZH, 1C0Q, 1C0R, 1C1U, 1C1V, 1C1W, 1C4D, 1C4U, 1C4V, 1C4Y, 1C5F, 1C5L, 1C5N, 1C5O, 1C9I, 1C9L, 1CA0, 1CA8, 1CA9, 1CBW, 1CE1, 1CE6, 1CF0, 1CFN, 1CFS, 1CFT, 1CG9, 1CHO, 1CJF, 1CJQ, 1CJR, 1CKA, 1CKB, 1CM4, 1CMI, 1CP3, 1CPI, 1CQ4, 1CU4, 1CVU, 1CWA, 1CWB, 1CWC, 1CWD, 1CWE, 1CWF, 1CWH, 1CWI, 1CWJ, 1CWK, 1CWL, 1CWM, 1CWO, 1CYN, 1CZI, 1CZY, 1CZZ, 1D01, 1D0J, 1D3D, 1D3P, 1D3Q, 1D3T, 1D4P, 1D4T, 1D4W, 1D5D, 1D5E, 1D5H, 1D5M, 1D5X, 1D5Z, 1D6E, 1D6W, 1D8D, 1D8E, 1D8T, 1D9I, 1DDV, 1DE7, 1DIT, 1DKD, 1DKX, 1DKY, 1DKZ, 1DLK, 1DM4, 1DN2, 1DOJ, 1DUY, 1DUZ, 1DVA, 1DWC, 1DWD, 1DWE, 1DXP, 1DY8, 1DY9, 1DZI, 1E27, 1E28, 1E4W, 1E4X, 1E6I, 1E8N, 1EAK, 1EB1, 1EBA, 1ED3, 1EDN, 1EE4, 1EE5, 1EEN, 1EEO, 1EEY, 1EEZ, 1EFG, 1EFX, 1EG4, 1EGP, 1EI8, 1EJ4, 1EJH, 1EJL, 1EJO, 1EJY, 1EKB, 1ELR, 1ELW, 1EMU, 1EOJ, 1EOL, 1EPL, 1EPM, 1ER8, 1EVH, 1F1J, 1F1W, 1F47, 1F4V, 1F59, 1F7A, 1F8A, 1F90, 1FBV, 1FCF, 1FEV, 1FFN, 1FFO, 1FFP, 1FG2, 1FGL, 1FIP, 1FIV, 1FIW, 1FJM, 1FKN, 1FN8, 1FO0, 1FPC, 1FPF, 1FPT, 1FRG, 1FV1, 1FVM, 1FY4, 1FY5, 1FYN, 1FYR, 1FYT, 1FZJ, 1FZK, 1FZM, 1FZO, 1G0Y, 1G1F, 1G1G, 1G1H, 1G1S, 1G30, 1G32, 1G37, 1G6G, 1G6R, 1G7P, 1G7Q, 1G9W, 1GA1, 1GA4, 1GA6, 1GAG, 1GBB, 1GBC, 1GBD, 1GBF, 1GBH, 1GBI, 1GBK, 1GBL, 1GBM, 1GDN, 1GDQ, 1GDU, 1GEC, 1GFF, 1GG6, 1GGD, 1GGI, 1GHB, 1GHG, 1GHV, 1GHW, 1GHX, 1GHY, 1GJ4, 1GJ5, 1GJ7, 1GMH, 1GMK, 1GO6, 1GTJ, 1GTL, 1GUL, 1GUX, 1GVK, 1GVU, 1GVX, 1GWQ, 1GWR, 1GX, 1GY3, 1GYB, 1H0G, 1H0I, 1H24, 1H25, 1H26, 1H27, 1H28, 1H8D, 1H8I, 1H9L, 1H9O, 1HAG, 1HAH, 1HAX, 1HAZ, 1HBT, 1HC9, 1HDT, 1HEF, 1HES, 1HGT, 1HH3, 1HH6, 1HH9, 1HHA, 1HHC, 1HHF, 1HHG, 1HHH, 1HHI, 1HHJ, 1HHK, 1HHU, 1HHY, 1HHZ, 1HI6, 1HIM, 1HJA, 1HLT, 1HOC, 1HPG, 1HQJ, 1HR8, 1HSA, 1HSB, 1HTE, 1HXE, 1HXF, 1HXY, 1I1F, 1I1Y, 1I3I, 1I3Z, 1I4F, 1I73, 1I7A, 1I7R, 1I7T, 1I7U, 1I8I, 1I8K, 1IAK, 1IAU, 1IFH, 1IHJ, 1IHS, 1IHT, 1IID, 1IKF, 1IM3, 1INQ, 1IQ1, 1IQ5, 1IR3, 1IS0, 1ITT, 1IWQ, 1IZE, 1J19, 1J2X, 1J4X, 1J71, 1J7Z, 1J80, 1J81, 1J82, 1J8H, 1JAC, 1JAN, 1JAP, 1JBU, 1JCR, 1JCS, 1JD5, 1JD6, 1JDP, 1JET, 1JEU, 1JEV, 1JF1, 1JG3, 1JGD, 1JGE, 1JHT, 1JK4, 1JK8, 1JN5, 1JP5, 1JPF, 1JPG, 1JPL, 1JQ8, 1JQ9, 1JRR, 1JRS, 1JRT, 1JUF, 1JUQ, 1JVQ, 1JWG, 1JWM, 1JWS, 1JWU, 1JXP, 1JXQ, 1JYQ, 1JYR, 1K21, 1K22, 1K2D, 1K3A, 1K4W, 1K5N, 1K8D, 1KAP, 1KBG, 1KC2, 1KC5, 1KCR, 1KCS, 1KDV, 1KDY, 1KDZ, 1KE1, 1KE2, 1KG0, 1KHP, 1KHQ, 1KJ2, 1KJ3, 1KJ4, 1KJ7, 1KJF, 1KJG, 1KJH, 1KJM, 1KJV, 1KKQ, 1KLG, 1KLU, 1KNA, 1KNE, 1KPR, 1KPU, 1KPV, 1KTR, 1KTS, 1KTT, 1KUG, 1KUI, 1KUK, 1KV6, 1KY6, 1KY7, 1KYC, 1KYD, 1KYF, 1KYU, 1KZO, 1KZP, 1L0A, 1L2I, 1L7Z, 1LB5, 1LB6, 1LCJ, 1LCK, 1LD9, 1LEG, 1LEK, 1LEW, 1LEZ, 1LF8, 1LHC, 1LHD, 1LHE, 1LHF, 1LHG, 1LJ2, 1LK2, 1LK6, 1LKK, 1LM8, 1LOP, 1LP9, 1LS5, 1LTJ, 1LTX, 1LU0, 1LVB, 1LVM, 1LYB, 1M05, 1M21, 1M24, 1M27, 1M43, 1M45, 1M46, 1M4H, 1M5N, 1M6O, 1M72, 1M7E, 1MA3, 1MCB, 1MCC, 1MCD, 1MCE, 1MCF, 1MCH, 1MCI, 1MCJ, 1MCK, 1MCL, 1MCN, 1MCQ, 1MCR, 1MCS, 1MF4, 1MFG, 1MFL, 1MHC, 1MHW, 1M15, 1MIK, 1MIZ, 1MK7, 1MK9, 1MPA, 1MT7, 1MT8, 1MT9, 1MTN, 1MU6, 1MU8, 1MUE, 1MV9, 1MVC, 1MVU, 1MWA, 1MXE, 1MZ, 1MN9, 1N12, 1N2R, 1N3N, 1N4H, 1N4M, 1N4P, 1N4Q, 1N4R, 1N4S, 1N51, 1N59, 1N5A, 1N5Z, 1N64, 1N7F, 1NAK, 1NAM, 1NB3, 1NB5, 1NES, 1NEX, 1NH0, 1NIW, 1NJT, 1NKK, 1NLN, 1NLT, 1NLU, 1NM6, 1NO9, 1NPO, 1NQ7, 1NRP, 1NRR, 1NRS, 1NS3, 1NT1, 1NTV, 1NU2, 1NU8, 1NVQ, 1NVR, 1NVS, 1NX0, 1NX1, 1NY2, 1NZL, 1NZQ, 1NZV, 1OO6,

1O0D, 1O2G, 1O5G, 1O6K, 1O6L, 1O6P, 1O9D, 1O9F, 1O9K, 1O9S, 1O9U, 1OAI, 1OBX, 1OBY, 1OBZ, 1OEB, 1OEX, 1OF2, 1OGA, 1OGT, 1OHE, 1OJ5, 1OK7, 1OKV, 1OKW, 1OKX, 1OL1, 1OL2, 1OLA, 1OLC, 1OM9, 1OOK, 1OQN, 1OR8, 1ORH, 1OSV, 1OSZ, 1OT5, 1OT7, 1OU8, 1OV3, 1OW8, 1OX1, 1OX9, 1OXG, 1OXN, 1OXQ, 1OY7, 1OYT, 1OZB, 1P02, 1P03, 1P04, 1P05, 1P06, 1P10, 1P11, 1P12, 1P13, 1P22, 1P4B, 1P4N, 1P4U, 1P7V, 1P7W, 1P8J, 1P93, 1P9U, 1PAD, 1PAU, 1PCG, 1PCX, 1PD0, 1PD1, 1PDQ, 1PEG, 1PEK, 1PFB, 1PFG, 1PIP, 1PIV, 1PJ8, 1PJM, 1PNJ, 1PPN, 1PO1, 1PO2, 1POP, 1PPG, 1PQ8, 1PSO, 1PTT, 1PTU, 1PU9, 1PUA, 1PVC, 1PWV, 1PY1, 1PYW, 1PYZ, 1PZ5, 1PZL, 1Q1A, 1Q1S, 1Q2C, 1Q2D, 1Q3L, 1Q3P, 1Q4K, 1Q4Q, 1Q7D, 1QBQ, 1QBV, 1QC6, 1QD6, 1QD8, 1QEWF, 1QGR, 1QHR, 1QIX, 1QJ1, 1QJ6, 1QJ7, 1QJA, 1QJB, 1QJJ, 1QKA, 1QKB, 1QKZ, 1QLF, 1QLS, 1QNG, 1QNH, 1QO3, 1QQD, 1QR1, 1QR3, 1QRN, 1QS8, 1QSE, 1QSF, 1QSN, 1QTX, 1QUR, 1QXA, 1QZ0, 1QZ2, 1R17, 1R1L, 1R1P, 1R1Q, 1R1R, 1R1S, 1R2B, 1R42, 1R4L, 1R5I, 1R5V, 1R5W, 1R64, 1R9N, 1RBC, 1RBD, 1RBE, 1RBF, 1RBG, 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1YY4, 1YY6, 1YYE, 1YYF, 1Z3L, 1Z3M, 1Z3P, 1Z71, 1Z7K, 1Z8G, 1ZAF, 1ZB5, 1ZBC, 1ZBK, 1ZBW, 1ZDT, 1ZDU, 1ZEA, 1ZFP, 1ZGI, 1ZGV, 1ZGY, 1ZH7, 1ZHB, 1ZHK, 1ZHL, 1ZKF, 1ZKY, 1ZM6, 1ZMI, 1ZMS, 1ZRB, 1ZSD, 1ZT1, 1ZT7, 1ZTZ, 1ZUK, 1ZUZ, 1ZVS, 1ZVZ, 1ZW2, 1ZY1, 1ZYS, 1ZZD, 2A25, 2A2X, 2A3I, 2A3Z, 2A6D, 2A6I, 2A6K, 2A83, 2ADV, 2AGE, 2AGG, 2AGI, 2AIJ, 2AIK, 2AK4, 2AKA, 2AMQ, 2AN6, 2ANK, 2AO6, 2AOF, 2AOH, 2AOI, 2AOJ, 2AOS, 2AP2, 2APH, 2ARQ, 2ARR, 2AST, 2ASU, 2AUC, 2AV1, 2AV7, 2AW6, 2AWW, 2AX3, 2AXF, 2AXG, 2AXI, 2AXZ, 2AZM, 2B05, 2B0S, 2B1J, 2B1N, 2B1V, 2B1Z, 2B23, 2B2U, 2B2V, 2B6N, 2B7F, 2B9H, 2B9I, 2B9J, 2BB4, 2BBA, 2BCD, 2BCK, 2BCX, 2BD2, 2BD3, 2BD4, 2BD5, 2BD7, 2BD8, 2BDA, 2BDX, 2BDY, 2BE1, 2BGR, 2BIL, 2BJ4, 2BNQ, 2BNR, 2BP3, 2BP5, 2BQZ, 2BR9, 2BRR, 2BSR, 2BSS, 2BST, 2BTP, 2BUO, 2BVO, 2BVP, 2BVQ, 2BVR, 2BVS, 2BXT, 2BXU, 2BZ8, 2BZK, 2BZW, 2C1J, 2C1N, 2C23, 2C3I, 2C5I, 2C5K, 2C5V, 2C5W, 2C63, 2C6W, 2C74, 2C77, 2C7U, 2C8W, 2C8X, 2C8Y, 2C8Z, 2C90, 2C93, 2CCH, 2CCI, 2CE8, 2CE9, 2CF8, 2CF9, 2CHN, 2CHO, 2CI9, 2CIA, 2CII, 2CIK, 2CK0, 2CKB, 2CLR, 2CLV, 2CLZ, 2CN0, 2CNM, 2CNX, 2CNZ, 2CO0, 2CO2, 2CV3, 2CVY, 2CWG, 2D0N, 2D10, 2D1X, 2D3G, 2D5W, 2DEW, 2DEX, 2DEY, 2DF6, 2DO2, 2DOH, 2DP4, 2DPQ, 2DPR, 2DQK, 2DRK, 2DRM, 2DRT, 2DRX, 2DS8, 2DUJ, 2DVQ, 2DVR, 2DVS, 2DWX, 2DXP, 2DYH, 2DYP, 2DZE, 2E3K, 2E7L, 2EAX, 2EGN, 2EH8, 2EMT, 2EPH, 2ER0, 2ER6, 2ER7, 2ER9, 2ESL, 2ESV, 2F31, 2F3Y, 2F49, 2F4O, 2F53, 2F54, 2F58, 2F5B, 2F69, 2F6J, 2F74, 2F8E, 2FAI, 2FDM, 2FEQ, 2FES, 2FF3, 2FF4, 2FF6, 2FFD, 2FFF, 2FFU, 2FGE, 2FIB, 2FIV, 2FKA, 2FLK, 2FLU, 2FLW, 2FMF, 2FMH, 2FMI, 2FMK, 2FNS, 2FNT, 2FNX, 2FO4, 2FO5, 2FOJ, 2FOO, 2FOP, 2FP7, 2FSA, 2FTS, 2FVJ, 2FWO, 2FX7, 2FX8, 2FX9, 2FYM, 2FYS, 2FYY, 2FZ3, 2G1T, 2G2F, 2G2L, 2G30, 2G3V, 2G44, 2G49, 2G58, 2G5B, 2G5O, 2G6Q, 2G83, 2G8Z, 2G99, 2G9A, 2G9H, 2GCH, 2GDC, 2GDE, 2GFA, 2GGM, 2GHQ, 2GHT, 2GIT, 2GJ6, 2GNS, 2GPH, 2GPO, 2GRL, 2GS6, 2GSI, 2GT9, 2GTK, 2GTW, 2GTZ, 2GUO, 2GV2, 2GWW, 2H13, 2H1C, 2H1P, 2H1U, 2H2D, 2H2F, 2H2G, 2H2H, 2H43, 2H4F, 2H4H, 2H4J, 2H59, 2H5D, 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3WOR, 3WP0, 3WP1, 3WS3, 3WS6, 3WSR, 3WT5, 3WT6, 3WT7, 3WTQ, 3WUT, 3WUU, 3WUV, 3WUU, 3WV0, 3WXA, 3X11, 3X12, 3X13, 3X14, 3X23, 3ZDF, 3ZDI, 3ZDY, 3ZDZ, 3ZE0, 3ZE1, 3ZE2, 3ZEV, 3ZG5, 3ZG6, 3ZGC, 3ZHA, 3ZHE, 3ZIL, 3ZIN, 3ZIO, 3ZIP, 3ZIQ, 3ZIR, 3ZKE, 3ZKF, 3ZMP, 3ZMV, 3ZMZ, 3ZN0, 3ZN1, 3ZO1, 3ZQ8, 3ZQF, 3ZQG, 3ZQH, 3ZQI, 3ZRJ, 3ZRZ, 3ZS6, 3ZVY, 3ZYB, 3ZZY, 3ZZZ, 4A0I, 4A0J, 4A0N, 4A1U, 4A1W, 4A1X, 4A2A, 4A4B, 4A4C, 4A5X, 4A62, 4A7J, 4AA1, 4AA2, 4ABI, 4ABJ, 4AEN, 4AFJ, 4AIF, 4AJY, 4AKT, 4AM9, 4AOM, 4APH, 4APJ, 4APO, 4APR, 4AR8, 4ARF, 4ASQ, 4ASR, 4AU2, 4AU3, 4AU7, 4AUC, 4AW9, 4AWA, 4AWB, 4AX9, 4AXY, 4AYV, 4AYY, 4AZ2, 4AZA, 4B18, 4B3B, 4B45, 4B4N, 4B60, 4B7E, 4B7T, 4B8O, 4B8P, 4B8Y, 4B9W, 4BA3, 4BAH, 4BAK, 4BAM, 4BAN, 4BAO, 4BAQ, 4BEA, 4BEY, 4BG6, 4BH7, 4BH8, 4BJT, 4BL0, 4BLB, 4BLD, 4BOS, 4BP9, 4BPI, 4BPJ, 4BPK, 4BQD, 4BQK, 4BT9, 4BTA, 4BTB, 4BU0, 4BU1, 4BUO, 4BUZ, 4BVE, 4BFV, 4BVG, 4BXF, 4BXR, 4BXW, 4C1Q, 4C2C, 4C2F, 4C33, 4C34, 4C35, 4C5A, 4C5I, 4C78, 4C7B, 4C93, 4C95, 4CAY, 4CC2, 4CC3, 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4FIM, 4FJP, 4FL5, 4FL8, 4FLG, 4FM6, 4FMN, 4FMQ, 4FN5, 4FOR, 4FQX, 4FR3, 4FTG, 4FTV, 4FVD, 4FVL, 4FVT, 4FYS, 4FYI, 4FZ3, 4G0D, 4G1C, 4G1D, 4G1W, 4G1Y, 4G1Z, 4G20, 4G21, 4G2H, 4G2Z, 4G35, 4G3B, 4G42, 4G43, 4G5G, 4G5Q, 4G69, 4G6A, 4G8G, 4G8I,

4G9D, 4G9F, 4GAG, 4GAJ, 4GBA, 4GBX, 4GCH, 4GEQ, 4GFU, 4GFV, 4GFF, 4GGD, 4GGN, 4GKN, 4GKS, 4GKV, 4GL8, 4GLD, 4GLR, 4GLY, 4GM8, 4GM9, 4GMB, 4GNE, 4GNF, 4GNG, 4GNT, 4GPL, 4GQ6, 4GRK, 4GRV, 4GS0, 4GVC, 4GVD, 4GVU, 4GW1, 4GW5, 4GW8, 4GXL, 4GY5, 4GYE, 4GYO, 4GYW, 4GYY, 4GZ3, 4GZF, 4H0H, 4H25, 4H26, 4H36, 4H39, 4H3B, 4H3H, 4H3K, 4H3P, 4H3Q, 4H4F, 4H75, 4HAB, 4HAN, 4HCZ, 4HD8, 4HDA, 4HDQ, 4HFZ, 4HGC, 4HH6, 4HHA, 4HKC, 4HKJ, 4HOM, 4HON, 4HP2, 4HPO, 4HPY, 4HQR, 4HRG, 4HRH, 4HS3, 4HS6, 4HS8, 4HT6, 4HTP, 4HTV, 4HUX, 4HVA, 4HVU, 4HVV, 4HW4, 4HWZ, 4HX1, 4HXJ, 4HY2, 4HY7, 4HY9, 4HYB, 4HY5, 4HZL, 4I1P, 4I2Z, 4I31, 4I32, 4I33, 4I48, 4I4W, 4I51, 4I5B, 4I5L, 4I5N, 4I7B, 4I7C, 4I7D, 4IA1, 4IA2, 4IA3, 4IA7, 4IB5, 4ICZ, 4IEA, 4IEL, 4IFI, 4IFL, 4IGA, 4IGK, 4IGQ, 4IHO, 4IIM, 4IIO, 4IJ8, 4IKA, 4IKN, 4IMI, 4IMJ, 4IMQ, 4IMZ, 4IN9, 4INH, 4IOI, 4IPZ, 4IS6, 4ISQ, 4ITZ, 4IU7, 4IUI, 4IUR, 4IUT, 4IUU, 4IUV, 4IV2, 4IV4, 4IVH, 4IVW, 4IVY, 4IW6, 4IW8, 4IWC, 4IWF, 4IZY, 4J1V, 4J24, 4J26, 4J2C, 4J2J, 4J44, 4J45, 4J46, 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4M55, 4M5T, 4M6E, 4M7C, 4M8E, 4M8H, 4M91, 4M92, 4MBE, 4MCY, 4MCZ, 4MD0, 4MD4, 4MD5, 4MDD, 4MDI, 4MDJ, 4MDR, 4MFL, 4MFp, 4MFQ, 4MG5, 4MG6, 4MG7, 4MG8, 4MG9, 4MGA, 4MGB, 4MGC, 4MGD, 4MJ5, 4MJ6, 4MJH, 4MJI, 4MLI, 4MLS, 4MN3, 4MNQ, 4MNV, 4MNW, 4MNX, 4MNY, 4MQV, 4MS8, 4MVK, 4MXQ, 4MZ5, 4MZ6, 4MZf, 4MZH, 4MZJ, 4MZK, 4MZL, 4N0C, 4N0Y, 4N39, 4N3A, 4N3W, 4N4F, 4N5T, 4N6P, 4N7G, 4N7H, 4N7Y, 4N84, 4N8C, 4N8V, 4NAQ, 4NB3, 4NE9, 4NEC, 4NF9, 4NGE, 4NGH, 4NHC, 4NIE, 4NM3, 4NM5, 4NM7, 4NMO, 4NMP, 4NMQ, 4NMR, 4NMS, 4NMT, 4NMV, 4NMx, 4NNd, 4NNL, 4NNM, 4NNX, 4NNy, 4NO0, 4NO2, 4NO3, 4NO5, 4NQV, 4NQX, 4NR1, 4NRX, 4NSK, 4NT6, 4NU8, 4NUF, 4NW2, 4NQX, 4NXR, 4NY3, 4NZ8, 4O1V, 4O21, 4O2C, 4O2E, 4O2F, 4O30, 4O36, 4O37, 4O3T, 4O42, 4O45, 4O46, 4O4Y, 4O51, 4O56, 4O62, 4O6F, 4O6W, 4O97, 4O9V, 4O9W, 4OAJ, 4OAR, 4OBD, 4OBF, 4OBG, 4OBH, 4OBJ, 4OBK, 4OC7, 4OD7, 4ODK, 4ODL, 4ODM, 4ODN, 4ODP, 4ODQ, 4OED, 4OEY, 4OEZ, 4OFR, 4OFU, 4OH4, 4OH5, 4OHA, 4OIH, 4OIL, 4OJF, 4OK1, 4OKB, 4OKF, 4OKT, 4OKW, 4OKX, 4OLM, 4OMC, 4OMD, 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5HUW, 5HUY, 5HVP, 5HVZ, 5HYN, 5HYQ, 5HYR, 5HYX, 5HZ0, 5HZ1, 5HZ3, 5I25, 5I2I, 5I6A, 5I70, 5I7Z, 5I8C, 5I8M, 5I8X, 5I9B, 5I9T, 5IAB, 5IAE, 5IAG, 5IAJ, 5IAR, 5IAS, 5IAW, 5IB1, 5IB2, 5IB3, 5IB4, 5IB5, 5IBC, 5IBP, 5IBR, 5IC3, 5IC6, 5ICK, 5ICV, 5ICY, 5ICZ, 5ID0, 5ID1, 5IEH, 5IEK, 5IFJ, 5IG7, 5IGO, 5IH2, 5II0, 5IJK, 5IM7, 5INC, 5IND, 5INZ, 5IOK, 5IOP, 5IQL, 5IQM, 5IQN, 5IQQ, 5IR1, 5IRO, 5ISZ, 5ITF, 5IUE, 5IV2, 5IVN, 5IVX, 5IVZ, 5IX1, 5IXQ, 5IXT, 5IYV, 5IYX, 5IZ0, 5IZ2, 5IZ6, 5IZ9, 5IZA, 5IZF, 5IZJ, 5IZU, 5J19, 5J31, 5J3T, 5J4T, 5J4X, 5J50, 5J51, 5J5X, 5J6H, 5J9S, 5JBQ, 5JBT, 5JCY, 5JEK, 5JEL, 5JEO, 5JER, 5JEZ, 5JF0, 5JFD, 5JFG, 5JFI, 5JFT, 5JGE, 5JHN, 5JIN, 5JIY, 5JJ0, 5JJY, 5JJZ, 5JLB, 5JLZ, 5JM1, 5JM4, 5JMM, 5JMO, 5JP2, 5JPF, 5QJ1, 5JR2, 5JR4, 5JR6, 5JWD, 5JWE, 5JWP, 5JXH, 5JXJ, 5JY0, 5JYQ, 5JZU, 5JZY, 5JZZ, 5K18, 5K4F, 5K6S, 5K86, 5K8Q, 5K99, 5K9S, 5KCC, 5KCD, 5KCE, 5KCF, 5KCT, 5KCU, 5KCW, 5KD9, 5KDS, 5KEZ, 5KGN, 5KJH, 5KKL, 5KLT, 5KMX, 5KOA, 5KOG, 5KR9, 5KRA, 5KRC, 5KRF, 5KRH, 5KRI, 5KRJ, 5KRL, 5KRM, 5KRO, 5KS9, 5KSA, 5KSB, 5KSU, 5KSV, 5KVM, 5KWN, 5KYN, 5KZP, 5KZT, 5L0Y, 5L11, 5L20, 5L23, 5L7E, 5L7G, 5L7H, 5L7K, 5L83, 5L8E, 5L9B, 5L9V, 5LA9, 5LAK, 5LAS, 5LAX, 5LB7, 5LCE, 5LEO, 5LGA, 5LHW, 5LI1, 5LJN, 5LM1, 5LM5, 5LMF, 5LMG, 5LPD, 5LPR, 5LRG, 5LRJ, 5LRK, 5LSF, 5LSO, 5LSW, 5LU1, 5LU2, 5LU8, 5LU9, 5LUG, 5LUM, 5LUZ, 5LV0, 5LVP, 5LX2, 5LXH, 5LXI, 5LY1, 5LY3, 5LYN, 5LYQ, 5M00, 5M01, 5M02, 5M35, 5M37, 5M5G, 5M5R, 5M5S, 5M5T, 5M5U, 5M5V, 5M61, 5M9E, 5M9N, 5M9O, 5MBW, 5MCO, 5MCQ, 5ME3, 5MEN, 5MEO, 5MEP, 5MEQ, 5MER, 5MFE, 5MFF, 5MFG, 5MFH, 5MFI, 5MFJ, 5MFK, 5MGX, 5MHC, 5MHI, 5MHL, 5MHM, 5MHN, 5MHO, 5MJ5, 5MJT, 5MJY, 5MK0, 5MK1, 5MK2, 5MK3, 5MK4, 5MKJ, 5MKU, 5MLO, 5MLS, 5MLW, 5MM6, 5MMW, 5MO3, 5MOC, 5MP3, 5MP5, 5MR8, 5MRW, 5MT6, 5MT7, 5MT8, 5MU0, 5MU2, 5MX7, 5MXO, 5MY4, 5MY9, 5MYK, 5MYO, 5MYX, 5MZL, 5MZN, 5N10, 5N1D, 5N1E, 5N1K, 5N1L, 5N1M, 5N1N, 5N1O, 5N1W, 5N1Y, 5N22, 5N32, 5N33, 5N36, 5N37, 5N39, 5N3A, 5N3B, 5N3C, 5N3D, 5N3E, 5N3F, 5N4B, 5N4N, 5N4O, 5N4R, 5N4U, 5N4V, 5N4X, 5N4Y, 5N4Z, 5N50, 5N51, 5N52, 5N5L, 5N5M, 5N5R, 5N5T, 5N5W, 5N6B, 5N74, 5N75, 5N7B, 5N7G, 5N7P, 5N7Q, 5N7U, 5N7X, 5N85, 5N91, 5N9H, 5N9I, 5N9P, 5NAF, 5NAS, 5NBL, 5NC2, 5NC7, 5ND0, 5NDT, 5NES, 5NEY, 5NFP, 5NFT, 5NFU, 5NIS, 5NI7, 5NI8, 5NI9, 5NIB, 5NIG, 5NIN, 5NJ9, 5NJA, 5NJC, 5NJJ, 5NJJ, 5NKP, 5NMA, 5NMB, 5NME, 5NMF, 5NMG, 5NMH, 5NMK, 5NNC, 5NND, 5NNE, 5NNF, 5NNG, 5NNP, 5NPH, 5NPI, 5NPJ, 5NPR, 5NPS, 5NPZ, 5NQ0, 5NQ1, 5NQ2, 5NQ3, 5NQA, 5NQV, 5NSC, 5NTJ, 5NTW, 5NUI, 5NW8, 5NWI, 5NWJ, 5NX1, 5NXQ, 5O0E, 5O0Z, 5O45, 5O4Y, 5O5M, 5O76, 5O8K, 5O9S, 5O9T, 5O9U, 5O9V, 5OAV, 5OB0, 5OB1, 5OB2, 5OBT, 5OCK, 5OCX, 5OCY, 5OGL, 5OJ5, 5OJR, 5OK3, 5OK6, 5OKC, 5OL0, 5OL3, 5ONA, 5ONJ, 5ONP, 5ONQ, 5ONR, 5OOB, 5OSI, 5OT3, 5OTG, 5OU8, 5OUA, 5OUC, 5OUS, 5OV3, 5OVC, 5OVP, 5OVV, 5OW5, 5OW7, 5OW9, 5OWD, 5OWP, 5OX2, 5OY3, 5PAD, 5Q0F, 5Q0I, 5Q0J, 5Q0K, 5Q0L, 5Q0M, 5Q0N, 5Q0O, 5Q0P, 5Q0Q, 5Q0R, 5Q0S, 5Q0T, 5Q0U, 5Q0V, 5Q0W, 5Q0X, 5Q0Y, 5Q0Z, 5Q10, 5Q11, 5Q12, 5Q13, 5Q14, 5Q15, 5Q16, 5Q17, 5Q18, 5Q19, 5Q1A, 5Q1B, 5Q1C, 5Q1D, 5Q1E, 5Q1F, 5Q1G, 5Q1H, 5Q1I, 5SGA, 5SUT, 5SVE, 5SVI, 5SVX, 5SVY, 5SVZ, 5SW9, 5SWF, 5SWQ, 5SSWS, 5SWZ, 5SXW, 5SXP, 5SYZ, 5SZB, 5SZC, 5T0K, 5T0M, 5T0Q, 5T1G, 5T1I, 5T1K, 5T1L, 5T1M, 5T1Z, 5T2S, 5T5J, 5T5L, 5T5O, 5T5P, 5T6J, 5T6P, 5T6W, 5T6X, 5T6Y, 5T6Z, 5T70,

5T78, 5T8R, 5TBD, 5TDA, 5TDB, 5TDC, 5TDD, 5TDR, 5TDW, 5TED, 5TEG, 5TEZ, 5TH2, 5TIL, 5TKJ, 5TKK, 5TLD, 5TLF, 5TLG, 5TLL, 5TLM, 5TLO, 5TLP, 5TLT, 5TLU, 5TLV, 5TLX, 5TLY, 5TM1, 5TM2, 5TM3, 5TM4, 5TM5, 5TM6, 5TM7, 5TM8, 5TM9, 5TML, 5TMM, 5TMO, 5TMQ, 5TMR, 5TMS, 5TMT, 5TNU, 5TMV, 5TMW, 5TMZ, 5TN1, 5TN3, 5TN4, 5TN5, 5TN6, 5TN7, 5TN8, 5TQ1, 5TQC, 5TQS, 5TTW, 5TU5, 5TU6, 5TWA, 5TWG, 5TWH, 5TWO, 5TXE, 5TXS, 5TYI, 5TZP, 5TZQ, 5U06, 5U1M, 5U1Q, 5U2D, 5U2J, 5U3N, 5U3O, 5U5C, 5U5F, 5U5M, 5U5P, 5U5R, 5U5T, 5U66, 5U6A, 5U6K, 5U98, 5UA5, 5UCL, 5UFS, 5UHR, 5UJT, 5UL6, 5ULO, 5UML, 5UMM, 5UMZ, 5UN8, 5UNJ, 5UUK, 5UUP, 5UW3, 5UW5, 5UW7, 5UWH, 5UWI, 5UWJ, 5UWM, 5UWO, 5UWP, 5UWQ, 5UWR, 5UWS, 5UWT, 5UWU, 5UWW, 5UY9, 5UZK, 5UZW, 5V1A, 5V1D, 5V1T, 5V1U, 5V1V, 5V1Y, 5V1Z, 5V21, 5V22, 5V2P, 5V2Q, 5V4B, 5V5L, 5V5M, 5V5O, 5V5P, 5V61, 5V62, 5V64, 5V6M, 5V6Y, 5V8K, 5V9P, 5VA6, 5VA9, 5VAB, 5VAC, 5VAH, 5VAO, 5VAP, 5VAQ, 5VAU, 5VB9, 5VBC, 5VBL, 5VCL, 5VGD, 5VGE, 5VHB, 5VI6, 5VI9, 5VIB, 5VIE, 5VIF, 5VK0, 5VK1, 5VKL, 5VLA, 5VLH, 5VLK, 5VLL, 5VLP, 5VNB, 5VNE, 5VNF, 5VNG, 5VNH, 5VNI, 5VNJ, 5VNK, 5VQI, 5VS7, 5VSG, 5VTB, 5VVT, 5VVU, 5VVV, 5VWX, 5VWI, 5VWK, 5VWX, 5VXR, 5VYO, 5VZ5, 5VZU, 5VZY, 5W3P, 5W4E, 5W4F, 5W4G, 5W4J, 5W67, 5W69, 5W6A, 5W7I, 5W7J, 5W7X, 5W7Y, 5W89, 5W93, 5WAI, 5WBH, 5WBJ, 5WE0, 5WES, 5WET, 5WEU, 5WFC, 5WGD, 5WGG, 5WGQ, 5WHH, 5WIR, 5WIE, 5WJN, 5WKF, 5WLE, 5WLG, 5WLI, 5WLJ, 5WMN, 5WMO, 5WMP, 5WMQ, 5WMR, 5WN9, 5WNB, 5WOU, 5WQD, 5WQL, 5WRD, 5WRI, 5WRJ, 5WRK, 5WRM, 5WSH, 5WTT, 5WUM, 5WUN, 5WWJ, 5WWU, 5WXC, 5WXF, 5WXG, 5WXH, 5WXN, 5WXO, 5WXP, 5WXQ, 5WXR, 5WY2, 5WYI, 5WZX, 5WZZ, 5X08, 5X3S, 5X54, 5X7B, 5X8N, 5X8Q, 5X8U, 5X8W, 5X94, 5XAD, 5XCO, 5XCQ, 5XCR, 5XCS, 5XCT, 5XCU, 5XCV, 5XHZ, 5XMF, 5XMM, 5XN3, 5XNV, 5XO2, 5XOF, 5XOQ, 5XOS, 5XOT, 5XOV, 5XPL, 5XPM, 5XPN, 5XPO, 5XPP, 5XPT, 5XRR, 5XS3, 5XTZ, 5XUP, 5XUQ, 5XVW, 5XW1, 5XW5, 5XW8, 5XW9, 5XWA, 5XWJ, 5XWL, 5XWR, 5XXK, 5XXQ, 5XY9, 5XYF, 5XZF, 5XZH, 5ZXZ, 5Y18, 5Y1U, 5Y20, 5Y21, 5Y4H, 5Y53, 5Y59, 5Y5A, 5Y7W, 5Y91, 5YAY, 5YBA, 5YBE, 5YBU, 5YC1, 5YC3, 5YC4, 5YCO, 5YD3, 5YD4, 5YD5, 5YD8, 5YE3, 5YE4, 5YF4, 5YGD, 5YGF, 5YIP, 5YIS, 5YKO, 5YL7, 5YP5, 5YP6, 5YPO, 5YPR, 5YRS, 5YT0, 5YU6, 5YV5, 5YVX, 5YY4, 5Z12, 5Z8L, 5ZNP, 5ZUT, 5ZVW, 5ZW6, 5ZWE, 5ZWF, 5ZWH, 5ZWI, 6AIF, 6AM5, 6AMT, 6AMU, 6ANN, 6APR, 6AR2, 6ASZ, 6AT0, 6AT5, 6AT9, 6ATF, 6ATI, 6ATV, 6ATZ, 6AU5, 6AVF, 6AVG, 6AVZ, 6AXK, 6AXL, 6AXP, 6AYN, 6AZK, 6AZL, 6AZM, 6AZT, 6B27, 6B3X, 6B5L, 6B5M, 6B5N, 6B5O, 6B5P, 6B5Q, 6B5R, 6B5S, 6B5T, 6B67, 6B74, 6B77, 6B8J, 6B9H, 6B9Y, 6BAE, 6BAH, 6BB4, 6BCD, 6BDV, 6BFJ, 6BFL, 6BFO, 6BG0, 6BG1, 6BG4, 6BGA, 6BGK, 6BGQ, 6BGR, 6BGS, 6BH9, 6BHA, 6BHD, 6BHE, 6BHG, 6BHH, 6BHI, 6BIJ, 6BIL, 6BIN, 6BIR, 6BIV, 6BIX, 6BIY, 6BIZ, 6BJ3, 6BJ8, 6BPI, 6BQB, 6BRA, 6BRS, 6BUU, 6BVB, 6BW3, 6BW4, 6BXQ, 6BYK, 6BZ3, 6BZ9, 6BZD, 6BZU, 6BZV, 6BZY, 6C0H, 6C0I, 6C0Y, 6C1Q, 6C1R, 6C4U, 6C52, 6CBI, 6CBP, 6CBZ, 6CCT, 6CCU, 6CD8, 6CD9, 6CDC, 6CDG, 6CDM, 6CD0, 6CDP, 6CEN, 6CF6, 6CG4, 6CIT, 6CO3, 6CPL, 6CPN, 6CPO, 6CQJ, 6CQL, 6CQN, 6CQQ, 6CWP, 6D0X, 6D1U, 6DCW, 6DM4, 6DUB, 6EI2, 6EIH, 6EJ7, 6EJ8, 6EJ9, 6EJA, 6EJB, 6EJC, 6EJD, 6EJE, 6EJL, 6EL6, 6EL7, 6EL9, 6ENB, 6EO8, 6EO9, 6EOP, 6EQV, 6EQW, 6EQX, 6ESN, 6EWW, 6EX9, 6EXJ, 6F08, 6F09, 6F4P, 6F4S, 6F5E, 6FAU, 6FAV, 6FAW, 6FBK, 6FBT, 6FBW, 6FBY, 6FC6, 6FCP, 6FCR, 6FCS, 6FEL, 6FHU, 6FI5, 6FKP, 6FKY, 6FLG, 6FMP, 6FMQ, 6FNZ, 6FO7, 6FO8, 6FO9, 6FOB, 6FOD, 6FQ4, 6FQC, 6FY3, 6GFX, 6GGM, 6GH1, 6GH4, 6GHN, 6GHP, 6GK7, 6GL1, 6GMR, 6GY5, 6H0E, 6H8P, 6H9O, 6LPR, 6RLX, 7GCH, 7HVP, 7INS, 7KME, 7LPR, 8GCH, 8HVP, 8KME, 8LPR, 8PCH, 9LPR

Table S2. The binding energetic components of PMI protein–protein, PMI protein–peptide segment, and PTI protein–peptide ligand interactions for the 23 PMI/PTI systems

PDB ^a	Peptide	Interaction type	Binding energetic component (kcal/mol)			
			ΔE_{int}	ΔG_{slv}	$-T\Delta S$	ΔG_{tot}
1AK4_D:A	⁴⁸⁶ VHAGPIAP ⁴⁹³	PMI protein–protein	-290.6	151	72.4	-67.2
		PMI protein–peptide segment	-142.4	90.3	30.7	-21.4
		PTI protein–peptide ligand	-117.3	57.2	46.2	-13.9
2SNI_I:E	⁵⁴ GTIVTMEYRI ⁶³	PMI protein–protein	-306.2	173.6	59.2	-73.4
		PMI protein–peptide segment	-162.7	101.0	34.1	-27.6
		PTI protein–peptide ligand	-145.4	77.2	49.2	-19.0
1AY7_B:A	³⁴ LDALWDCLTG ⁴³	PMI protein–protein	-378.2	247.9	46.1	-84.2
		PMI protein–peptide segment	-177.8	127.8	19.3	-30.5
		PTI protein–peptide ligand	-160.6	109.6	25.6	-25.4
2C7M_A:B	⁵¹ QIQEDWELAERLQREE ⁶⁶	PMI protein–protein	-476.0	349.3	38.4	-88.3
		PMI protein–peptide segment	-388.2	311.0	22.3	-54.9
		PTI protein–peptide ligand	-357.4	281.6	29.6	-46.2
3FP6_I:E	¹¹ TGPCKKARI ¹⁹	PMI protein–protein	-347.2	251.1	47.2	-48.9
		PMI protein–peptide segment	-158.6	121.8	21.6	-15.2
		PTI protein–peptide ligand	-116.3	75.9	30.8	-9.6
3L4F_D:ABC	⁶⁴⁰ AWDETNL ⁶⁴⁶	PMI protein–protein	-268.9	159.2	57.3	-52.4
		PMI protein–peptide segment	-150.3	110.5	21.8	-18.0
		PTI protein–peptide ligand	-132.7	82.9	39.6	-10.2
1UEL_B:A	²⁸³ EEEQIAYAMQMSLQGA ²⁹⁸	PMI protein–protein	-258.4	148.5	47.2	-62.7
		PMI protein–peptide segment	-184.9	125.1	24.6	-35.2
		PTI protein–peptide ligand	-163.0	105.8	28.9	-28.3
1GH6_A:B	⁹⁹ NEENLFCSEEMP ¹¹⁰	PMI protein–protein	-265.4	149.3	72.4	-43.7
		PMI protein–peptide segment	-135.0	76.4	43.0	-15.6
		PTI protein–peptide ligand	-112.7	46.1	57.9	-8.7

			PMI protein–protein	-518.4	355.1	75.4	-87.9
2HLE_B:A	¹⁰⁶ QDIKFTIKFQEFSNLWGLE ¹²⁵	PMI protein–peptide segment	-273.2	216.8	28.0	-28.4	
		PTI protein–peptide ligand	-224.3	158.5	54.6	-11.2	
		PMI protein–protein	-385.9	249.4	72.0	-64.5	
2FD6_A:U	¹⁹ CVSNKYFSNIHWCN ³²	PMI protein–peptide segment	-266.1	194.0	45.2	-26.9	
		PTI protein–peptide ligand	-227.6	153.8	58.4	-15.4	
		PMI protein–protein	-207.8	122.1	42.0	-43.7	
1D6R_I:A	¹¹ QCACTKSNPPQ ²¹	PMI protein–peptide segment	-156.0	110.9	26.5	-18.6	
		PTI protein–peptide ligand	-129.4	73.6	47.3	-8.5	
		PMI protein–protein	-357.3	256.8	54.2	-46.3	
1GHQ_B:A	⁸¹ YKIRGSTP ⁸⁸	PMI protein–peptide segment	-188.2	154.8	18.7	-14.7	
		PTI protein–peptide ligand	-124.3	80.1	38.9	-5.3	
		PMI protein–protein	-212.7	116.3	57.5	-38.9	
1E6J_P:HL	²⁰⁴ ALGPAATLEEMMTA ²¹⁷	PMI protein–peptide segment	-158.4	99.2	44.9	-14.3	
		PTI protein–peptide ligand	-123.9	64.3	52.6	-7.0	
		PMI protein–protein	-375.6	270.9	37.3	-67.4	
1E96_A:B	²¹ ISYTTNAFPGE ³¹	PMI protein–peptide segment	-286.5	243.9	19.0	-23.6	
		PTI protein–peptide ligand	-207.1	152.7	43.9	-10.5	
		PMI protein–protein	-297.8	207.4	43.1	-47.3	
2I25_N:L	⁸⁶ ESRYGSYD ⁹³	PMI protein–peptide segment	-143.7	107.5	17.6	-18.6	
		PTI protein–peptide ligand	-106.5	65.4	32.7	-8.4	
		PMI protein–protein	-156.8	81.1	48.3	-27.4	
1AVX_B:A	⁵⁶¹ PYRIRF ⁵⁶⁶	PMI protein–peptide segment	-97.4	62.7	25.7	-9.0	
		PTI protein–peptide ligand	-72.0	33.9	34.9	-3.2	
		PMI protein–protein	-178.4	100.6	28.5	-49.3	
2OOB_A:B	⁹³³ DAKIAKLMG ⁹⁴¹	PMI protein–peptide segment	-132.0	91.5	15.9	-24.6	
		PTI protein–peptide ligand	-115.9	72.9	23.6	-19.4	

			PMI protein–protein	-227.4	135.6	40.9	-50.9
1A2K_E:B	²⁰³ VAQTTALPDE ²¹²		PMI protein–peptide segment	-182.5	125.7	27.3	-29.5
			PTI protein–peptide ligand	-143.7	94.7	36.7	-12.3
			PMI protein–protein	-317.2	203.3	48.9	-65.0
7CEI_B:A	⁵¹⁴ SRNNNNDRMKVGKAPKTRT ⁵³¹		PMI protein–peptide segment	-204.5	148.2	27.6	-28.7
			PTI protein–peptide ligand	-179.3	125.5	40.3	-13.5
			PMI protein–protein	-117.5	74.2	24.1	-19.2
1KTZ_B:A	⁴⁹ SITSICE ⁵⁵		PMI protein–peptide segment	-74.2	53.6	13.2	-7.4
			PTI protein–peptide ligand	-32.6	3.7	27.6	-1.3
			PMI protein–protein	-202.0	117.9	38.9	-45.2
2MTA_C:A	⁶⁷ GKIGPGLNDAYWT ⁷⁹		PMI protein–peptide segment	-135.4	92.7	24.8	-17.9
			PTI protein–peptide ligand	-99.3	36.4	52.4	-10.5
			PMI protein–protein	-398.5	254.5	96.4	-47.6
4MLF_D:B	³⁴⁶ PKPQSHNDGDFEEIPEEYLQ ³⁶⁵		PMI protein–peptide segment	-287.8	214.5	54.6	-18.7
			PTI protein–peptide ligand	-239.0	143.6	83.0	-12.4
			PMI protein–protein	-275.9	228.1	19.3	-28.5
4JLR_S:HL	⁶⁵ SELLSKINDMPITNDQKKLMSNDVL ⁸⁹		PMI protein–peptide segment	-214.7	186.0	11.4	-17.3
			PTI protein–peptide ligand	-198.3	168.8	16.8	-12.7

^aPDB_M1:M2: the PDB code of a PMI crystal structure and the complex members (M1 and M2) involved in the PMI. The first member M1 is the parent protein of peptide segment, and the second member M2.

Figures S1–S4

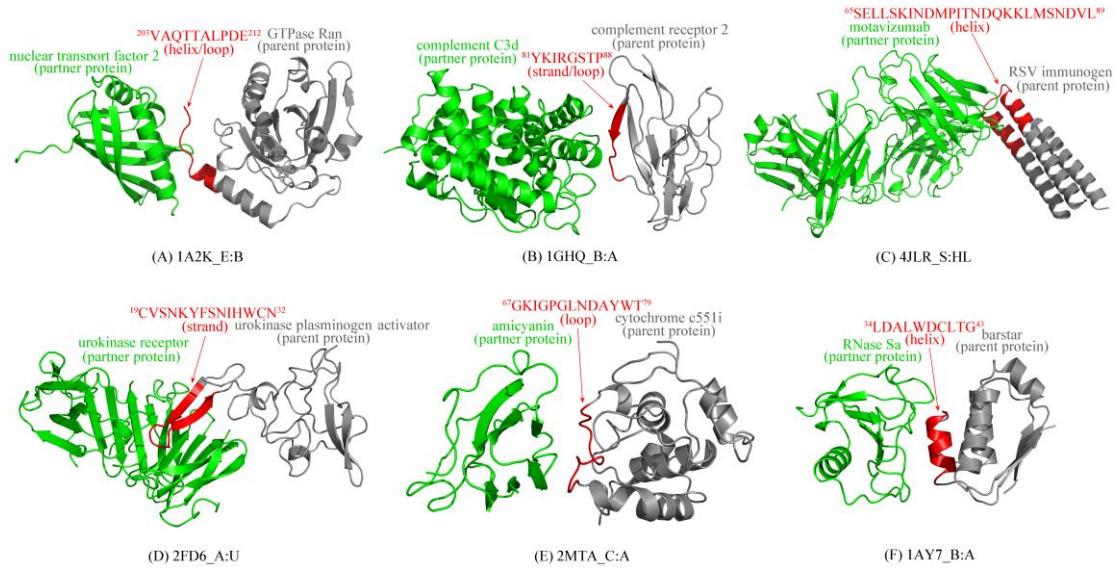


Figure S1. Some examples of PMIs investigated in this study. The partner protein is in green, and the parent protein is colored by red (peptide segment) and grey (protein context).

- (A) Nuclear transport factor 2–GTPase Ran complex (PDB: 1A2K_E:B).
- (B) Complement C3d–complement receptor 2 complex (PDB: 1GHQ_B:A).
- (C) Motavizumab–RSV immunogen complex (PDB: 4JLR_S:HL).
- (D) Urokinase receptor–urokinase plasminogen activator complex (PDB: 2FD6_A:U).
- (E) Amicyanin–cytochrome c551i complex (PDB: 2MTA_C:A). (F) RNase Sa–barstar complex (PDB: 1AY7_B:A).

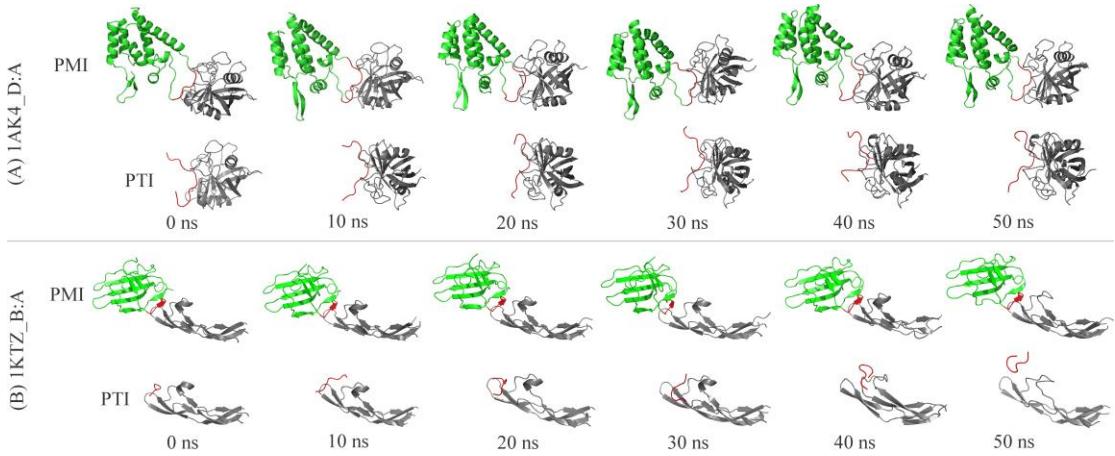


Figure S2. Comparison of the conformational snapshots of two PMI systems and their PTI counterparts separately extracted at the 0, 10, 20, 30, 40 and 50 ns of MD simulations.

- (A) The functional peptide segment in the PMI system 1AK4_D:A is a typical loop region that can tightly bind to its partner protein. A small conformational variation of the peptide segment is observed during the simulations of intact PMI system. In contrast, the conformational variation increases significantly when splitting the peptide segment from its parent context and re-performing simulations of the resulting PTI counterpart.
- (B) The functional peptide segment in the PMI system 1KTZ_B:A is a single β -strand that weakly touches on a hairpin region of its partner protein. A small conformational variation of the peptide segment is observed during the simulations of intact PMI system. However, the peptide exhibits a large conformational disorder and is gradually unbound from its partner protein when splitting the peptide segment from its parent context and re-performing simulations of the resulting PTI counterpart.

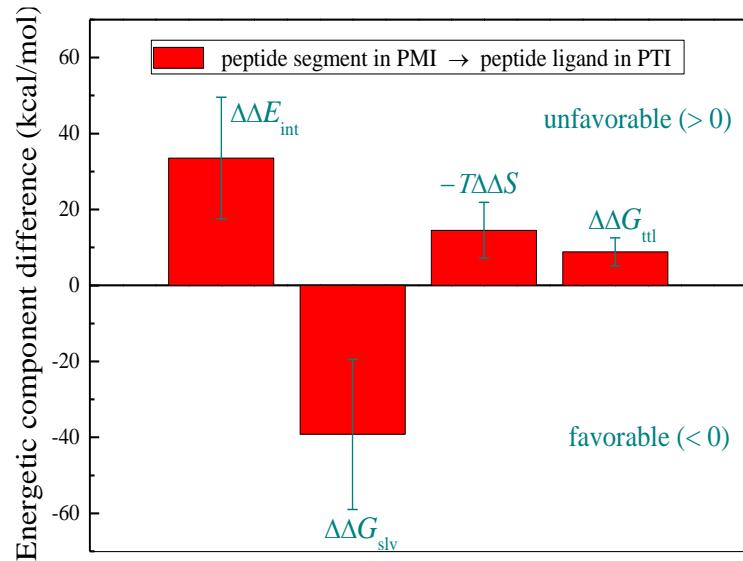


Figure S3. The average value and standard error (*a.v. $\pm s.e.$*) of differences of interaction energy ($\Delta\Delta E_{int}$), solvent effect ($\Delta\Delta G_{slv}$), entropy penalty ($-T\Delta\Delta S$), and total binding energy ($\Delta\Delta G_{ttl}$) between PMI peptide segment and PTI peptide ligand over the 23 PMI/PTI systems.

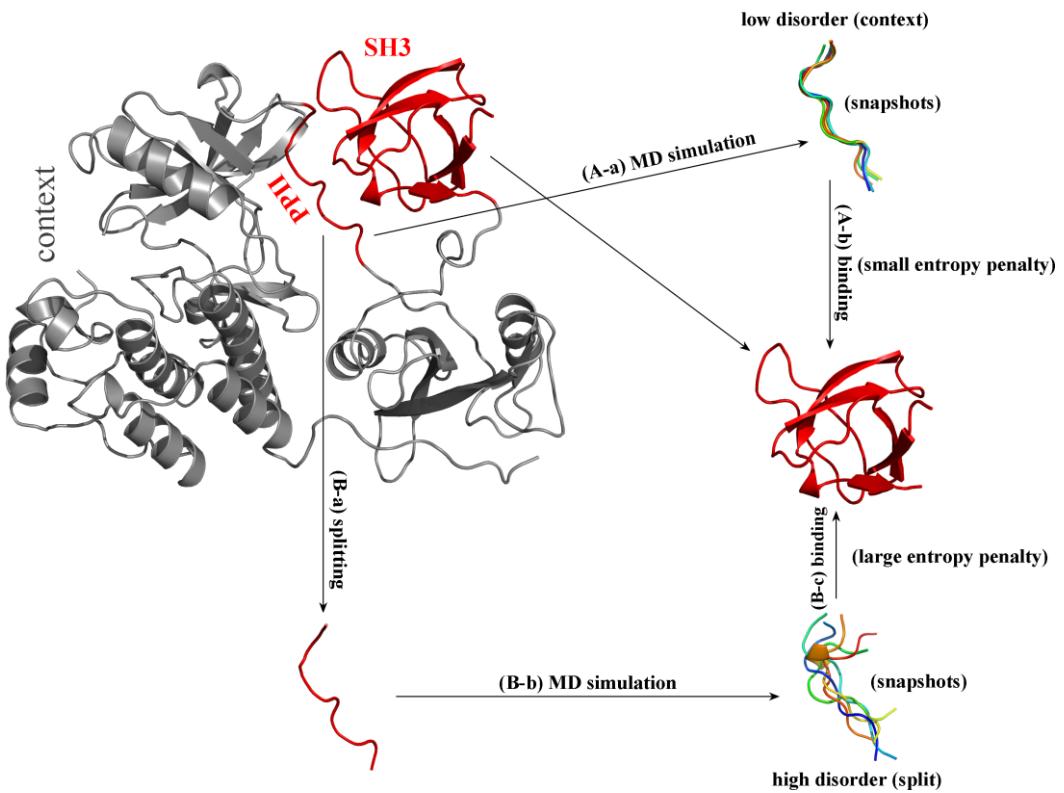


Figure S4. Schematic representation of context effect on SH3–PPII binding. The whole Scr kinase was subjected to 100-ns MD simulations (A-a), during which the PPII peptide segment (within the protein context) exhibits low disorder and its conformation was constrained around native state, thus incurring a small entropy penalty upon binding to SH3 domain (A-b). In contrast, the PPII peptide was split from the context as an isolated peptide ligand (B-a), which possesses a high intrinsic disorder when re-subjected to 100-ns MD simulations (B-b), and hence incurring a large entropy penalty upon binding to SH3 domain (B-c).