

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: ≤ 3 Å;
 - (iv) Number of chains in biological assembly: ≥ 2 ;
 - (v) Length of at least one chain: 5–30;
 - (vi) Sequence identity: $\leq 30\%$.
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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, 1A1X, 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, 1FIJ, 1FIW, 1F47, 1F4V, 1F59, 1F7A, 1F8A, 1F90, 1FBV, 1FCH, 1FEV, 1FFN, 1FFO, 1FFP, 1FG2, 1FGL, 1FIP, 1FIV, 1FIW, 1FJM, 1FKN, 1FN8, 1FO0, 1FPC, 1FPH, 1FPR, 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, 1GXC, 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, 1I31, 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, 1LKL, 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, 1MI5, 1MIK, 1MIZ, 1MK7, 1MK9, 1MPA, 1MT7, 1MT8, 1MT9, 1MTN, 1MU6, 1MU8, 1MUE, 1MV9, 1MVC, 1MVU, 1MWA, 1MXE, 1MZN, 1N0W, 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, 1O06,

100D, 102G, 105G, 106K, 106L, 106P, 109D, 109F, 109K, 109S, 109U, 10AI, 10BX, 10BY, 10BZ, 10EB, 10EX, 10F2, 10GA, 10GT, 10HE, 10J5, 10K7, 10KV, 10KW, 10KX, 10L1, 10L2, 10LA, 10LC, 10M9, 10OK, 10QN, 10R8, 10RH, 10SV, 10SZ, 10T5, 10T7, 10U8, 10V3, 10W8, 10X1, 10X9, 10XG, 10XN, 10XQ, 10Y7, 10YT, 10ZB, 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, 1PJN, 1PJP, 1PN3, 1PNV, 1PO1, 1PO2, 1POP, 1PPG, 1PQ8, 1PSO, 1PTT, 1PTU, 1PU9, 1PUA, 1PVC, 1PDW, 1PDZ, 1PY1, 1PYW, 1PYZ, 1PZ5, 1PZL, 1Q1A, 1Q1S, 1Q2C, 1Q2D, 1Q3L, 1Q3P, 1Q4K, 1Q4Q, 1Q7D, 1QBQ, 1QBV, 1QC6, 1QD6, 1QD8, 1QEW, 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, 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1YTI, 1YUC, 1YVH, 1YVL, 1YWO, 1YWT, 1YY4, 1YY6, 1YYE, 1YYP, 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, 2FMM, 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, 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2ORZ, 2OS2, 2OT7, 2OTU, 2OTW, 2OVH, 2OVM, 2OVQ, 2OVR, 2OX0, 2OXW, 2OXZ, 2OY2, 2OYH, 2OYI, 2P0R, 2P0W, 2P15, 2P1N, 2P1O, 2P1Q, 2P1T, 2P1U, 2P1V, 2P2T, 2P4R, 2P54, 2P5B, 2P5E, 2P5W, 2P6B, 2P8L, 2P8M, 2P8O, 2P8P, 2PAV, 2PB8, 2PBK, 2PC4, 2PCU, 2PEH, 2PEM, 2PHK, 2PIE, 2PKL, 2PKS, 2PL9, 2PLX, 2PMC, 2PNX, 2POY,

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4OLM, 4OMC, 4OMD, 4ONF, 4ONI, 4OO6, 4ORE, 4OS1, 4OS2, 4OS4, 4OS5, 4OS6, 4OS7, 4OU3, 4OUC, 4OV5, 4OWF, 4OXD, 4OY5, 4OYK, 4OZ1, 4OZ6, 4OZF, 4OZG, 4OZH, 4P02, 4P0A, 4P0B, 4P20, 4P3W, 4P6J, 4P6W, 4P6X, 4P9V, 4P9Z, 4PBZ, 4PD1, 4PES, 4PG2, 4PG9, 4PGB, 4PGC, 4PGD, 4PGE, 4PID, 4PIE, 4PIQ, 4PIS, 4PJZ, 4PK0, 4PK2, 4PK3, 4PL6, 4PLD, 4PLE, 4PLI, 4PLL, 4PN1, 4PO2, 4PO7, 4POH, 4POJ, 4PP3, 4PP5, 4PP6, 4PPP, 4PPS, 4PR5, 4PRA, 4PRB, 4PRD, 4PRE, 4PRH, 4PRI, 4PRN, 4PRP, 4PRY, 4PRZ, 4PS0, 4PS1, 4PSI, 4PSX, 4PV8, 4PV9, 4PXF, 4PXM, 4PYU, 4PYW, 4PZ3, 4PZ5, 4PZ6, 4Q0A, 4Q0X, 4Q13, 4Q1L, 4Q4I, 4Q6F, 4Q6H, 4Q6S, 4Q8D, 4Q94, 4Q96, 4QA5, 4QA6, 4QA7, 4QBM, 4QBQ, 4QBR, 4QBS, 4QC1, 4QC3, 4QE6, 4QE8, 4QH7, 4QH8, 4QJ2, 4QJ6, 4QJ7, 4QJ8, 4QJ9, 4QJA, 4QJR, 4QK4, 4QKC, 4QLI, 4QNZ, 4QO0, 4QO2, 4QOK, 4QPP, 4QQ4, 4QQI, 4QQM, 4QRP, 4QRQ, 4QRR, 4QRS, 4QRT, 4QRU, 4QSY, 4QT7, 4QTX, 4QTY, 4QU0, 4QU5, 4QU8, 4QU9, 4QUA, 4QUB, 4QUD, 4QUF, 4QUH, 4QUJ, 4QUI, 4QUJ, 4QUJ, 4QUM, 4QUT, 4QUU, 4QVF, 4QWN, 4QX7, 4QX8, 4QXB, 4QXC, 4QXH, 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4WNE, 4WNN, 4WPF, 4WPH, 4WQP, 4WRQ, 4WSF, 4WU5, 4WU7, 4WV6, 4WVD, 4WVH, 4WVI, 4WVJ, 4WVP, 4WVS, 4WVT, 4WVU, 4WX4, 4WX6, 4WX7, 4WY7, 4WYU, 4WZ9, 4WZX, 4X0W, 4X1H, 4X1N, 4X1P, 4X1Q, 4X1R, 4X1S, 4X1V, 4X2H, 4X2O, 4X34, 4X3E, 4X3G, 4X3H, 4X3I, 4X3K, 4X3O, 4X3P, 4X3S, 4X5K, 4X5W, 4X6N, 4X6S, 4X8N, 4X8P, 4X9R, 4X9V, 4X9W, 4XAI, 4XAL, 4XAW, 4XBE, 4XBU, 4XC1, 4XC2, 4XC3, 4XCF, 4XEE, 4XEF, 4XEK, 4XES, 4XEV, 4XFO, 4XGZ, 4XH2, 4XHV, 4XI7, 4XIB, 4XMH, 4XNH, 4XO9, 4XOA, 4XOB, 4XOD, 4XOE, 4XOJ, 4XPD, 4XSS, 4XST, 4XT9, 4XVJ, 4XXC, 4XXD, 4XYN, 4XZ1, 4Y19, 4Y1C, 4Y1D, 4Y29, 4Y2G, 4Y32, 4Y3B, 4Y3O, 4Y5I, 4Y6L, 4Y6O, 4Y7R, 4Y9W, 4YDV, 4YEC, 4YES, 4YGW, 4YGX, 4YGY, 4YH1, 4YI0, 4YJE, 4YJL, 4YK6, 4YL6, 4YNK, 4YNL, 4YO0, 4YOS, 4YOZ, 4YR6, 4YSI, 4YV8, 4YV9, 4YXB, 4YY6, 4YYD, 4YYG, 4YYH, 4YYI, 4YYJ, 4YYK, 4YYM, 4YYN, 4YZ6, 4YZH, 4Z09, 4Z0D, 4Z0E, 4Z0F, 4Z0R, 4Z0U, 4Z0X, 4Z0Y, 4Z0Z, 4Z10, 4Z20, 4Z2P, 4Z2V, 4Z33, 4Z5W, 4Z61, 4Z63, 4Z64, 4Z68, 4Z76, 4Z77, 4Z78, 4Z7N, 4Z7O, 4Z7Q, 4Z7U, 4Z7V, 4Z7W, 4Z88, 4Z89, 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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	486VHAGPIAP 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	54GTIVTMEYRI 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	34LDALWDCLTG 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	51QIQEDWELAERLQREE 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	11TGPCKARII 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	640AWDETNL 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	283EEEQIAYAMQMSLQGA 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	99NEENLFCSEEMP 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

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

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

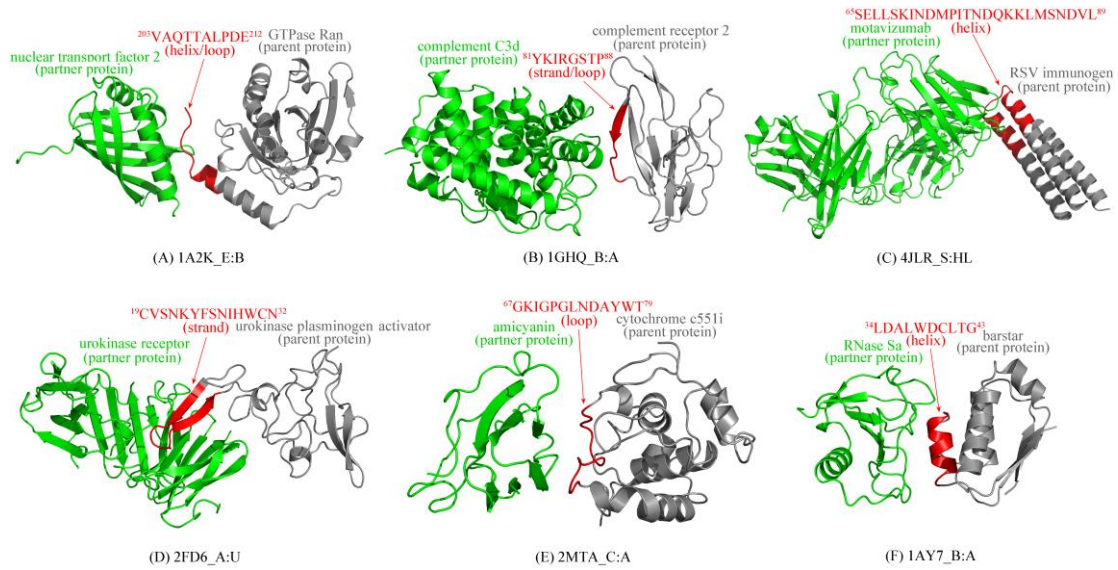


Figure S1. Some examples of PMIs investigated in this study. The partner protein is in green, and the parent protein is colored by red (peptide segment) and grey (protein context).

(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).

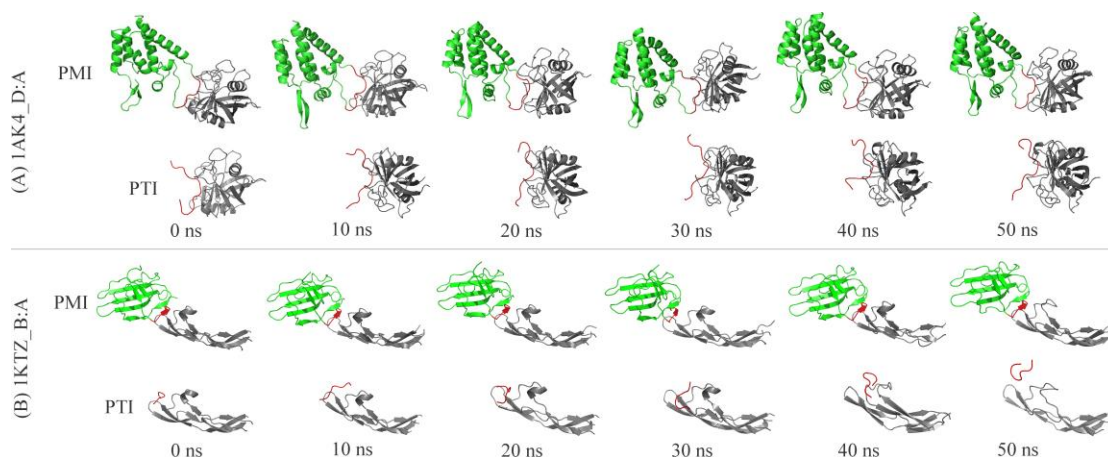


Figure S2. Comparison of the conformational snapshots of two PMI systems and their PTI counterparts separately extracted at the 0, 10, 20, 30, 40 and 50 ns of MD simulations.

- (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.

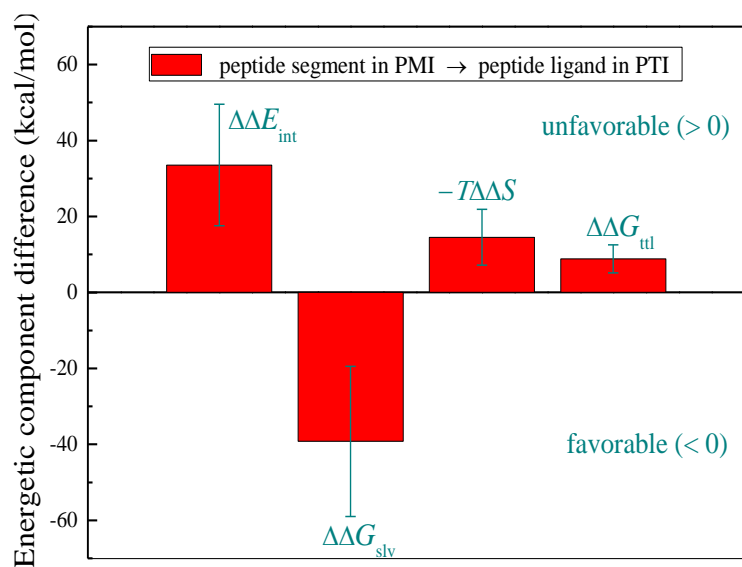


Figure S3. The average value and standard error (*a.v.* \pm *s.e.*) of differences of interaction energy ($\Delta\Delta E_{\text{int}}$), solvent effect ($\Delta\Delta G_{\text{slv}}$), entropy penalty ($-T\Delta\Delta S$), and total binding energy ($\Delta\Delta G_{\text{tot}}$) between PMI peptide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

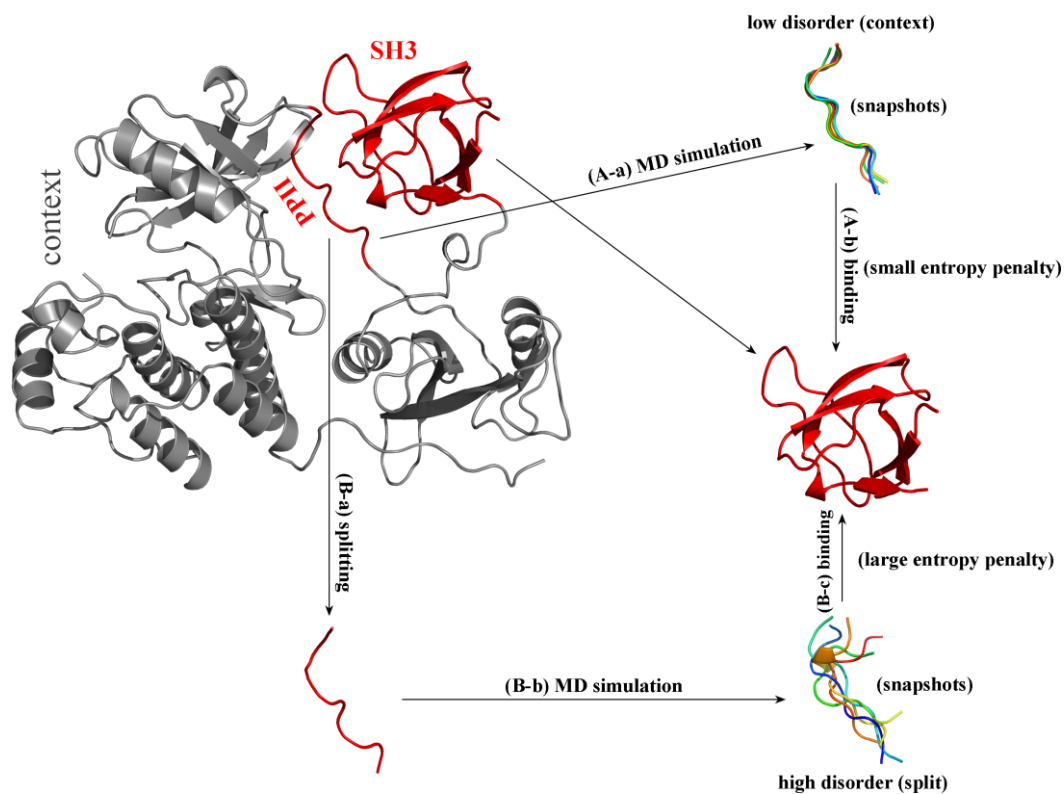


Figure S4. Schematic representation of context effect on SH3–PPII binding. The whole Scr kinase was subjected to 100-ns MD simulations (A-a), during which the PPII peptide segment (within the protein context) exhibits low disorder and its conformation was constrained around native state, thus incurring 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).