

Train/Val/Test splits. Lists of Mega-scale dataset “Dataset 2 (for ΔG ML)” wildtypes (WT) domains used in this study.

Split	WT domains
Train	<p>1OPS, 3V1A, EA_run7_1572_0002, EHEE_rd4_0086, 6RO9, 2I5L, 5Z2S, 1JIC, 2AME, 1ZHC, XX_run7_0974_0003, EHEE_rd4_0325, 1YU5, 2N9L, EEHEE_rd3_1716, EEHEE_rd4_0470, 9AME, 2MI6, 4UZW, 5KPH, GG_run5_0637_0006, EHEE_rd4_0098, 1UCS, EEHEE_rd4_0308, 2KVT, r10_437_TrROS_Hall, EEHEE_rd4_0003, 1AOY, 2L7M, EEHEE_rd3_1702, 2MC5, 2LXK, EHEE_rd2_1106, 2GP8, 1W4G, 7BPM, 5UP5, 6NMW, 1PGX, XX_run1_0254_0003, 3MYC, HEEH_KT_rd6_0280, 1H8K, 2RJV, EHEE_rd4_0864, EEHEE_rd3_0146, 2KT8, EHEE_rd2_0152, r11_233_TrROS_Hall, v2K43S_2KVV, HEEH_KT_rd6_3546, EEHEE_rd4_0481, 7MSI, 5FWB, EHEE_rd1_0459, 5JRT, v2_2L15, 1O6X, 2LUM, EEHEE_rd3_0657, 2M8E, 2JVD, 6MSI, HHH_rd1_0606, 6M3N, 2JTV, 2WQG, r6_560_TrROS_Hall, 2MWB, EEHEE_rd3_1367, 2N4R, 6AME, 1ORC, 2AMI, EEHEE_rd4_0763, HHH_rd1_0516, 2MKY, r4_43_TrROS_Hall, v2_2M5A, HHH_rd1_0598, 2HBB, HEEH_KT_rd6_0872, 4AME, EEHEE_rd3_1498, EHEE_rd2_1257, EHEE_rd4_0625, 2MKX, 2M0Y, 2L09, GG_run2_0085_0001, EHEE_rd4_0840, 2M2L, 2KFV, 2MYX, 2JWS, EEHEE_rd4_0371, 2JZ2, EEHEE_rd4_0794, XX_run10_1081_0004, 2KZJ, 2M0C, 4G3O, 1TUD, 2K5N, EHEE_rd4_0502, EHEE_rd2_0487, GG_run5_1309_0004, 1QLY, 5FW9, 2O2W, EHEE_rd1_0407, 3CQT, 1K1V, XX_run1_0455_0002, EEHEE_rd3_0809, 2L7F, 5VNT, 1S1N, 2LHC, 2MCH, XX_run5_0690_0002, 4UR4, EHEE_rd4_0394, XX_run8_1098_0003, XX_run5_1034_0004, 5XR0, v2_2LXE, HHH_rd1_0335, 5OAO, 2QFF, HEEH_rd4_0349, EHEE_rd3_0053, 2N88, 2YSB, 1PWT, 3I35, 2KYB, EEHEE_rd3_1818, 2LP5, 1B7J, 5LWC, 7JJK, GG_run4_1050_0002, 6FVC, 5UBS, 2D1U, v2_6IVS, 1MSJ, 1Y0M, 2CJJ, 5GU9, 3QF6, EA_run6_1429_0006, 5ECA, HHH_rd1_0493, 6NS8, 1EOL, EHEE_rd4_0463, 2M8U, EEHEE_rd3_0602, HEEH_KT_rd6_0007, HHH_rd4_0870, 6OBK, 2LX2, 2RRU, EHEE_rd4_0195, 2EXD, 1UFM, 2L6Q, r11_951_TrROS_Hall, XX_run8_1063_0003, r10_490_TrROS_Hall, 2L9R, EEHEE_rd4_0469, 2JWT, 5UYO, 8AME, 2K52, 1VII, 3L1X, 1IGV, 5UB0, 2JT1, 2ZW1, 2MCK, EEHEE_rd4_0647, EEHEE_rd3_0094, EEHEE_rd4_0363, 2KRU, 2MH8, 2L2P, 2MSJ, 1GJS, HEEH_rd3_0055, EEHEE_rd4_0256, 2KRS, 2KZI, HHH_rd1_0473, 1SRM, 2JVG, EEHEE_rd4_0784, 8MSI, HEEH_rd3_0223, 2ROT, 2MWA, 3NGP, 2B89, 2M8I, 1ZLM, 1GB4, 6IWS, 2LHR, r6_831_TrROS_Hall, GG_run3_1365_0003, EHEE_rd2_0372, 1MJC, 1EM7, 2LCL, EHEE_rd4_0726, EHEE_rd4_0044, EHEE_rd3_0035, 2LYR, 2MXD, 2K2A, v2_2HDZ, EHEE_rd2_0196, 2B88, EHEE_rd2_0601, HHH_rd1_0578, 1H92, 2CDT, HHH_rd4_0816, 1BK2, 1TGO, HEEH_rd4_0097, 2LJ3, 6IPY, EEHEE_rd3_1587, 1YP5, 1I2T, XX_run8_0733_0006, r7_587_TrROS_Hall, EEHEE_rd3_0019, 1IGD, XX_run1_0367_0004, EA_run5_0050_0004, 1QKX, 3AME, 1BNZ, 4HCK, 2LO1, HHH_rd2_0155, 1A0N, r16_88_TrROS_Hall, 2LYQ, 2M8J, 5AHT, GG_run3_1315_0003, 2M2J, 1LP1, 1UZC, 1YRF, 6NJF, 2M6Y, 1IFY, 2RRT, 2LSS, 2MA4, 1EKL, 1ENH, 6YSE, 2L2D, 2KR3, 6SCW, 1GL5, 2LYP, 1R69, 2KGT, 2LGW, 2KCM, EHEE_rd2_0751, GG_run1_1390_0006, EA_run2_0325_0005, EEHEE_rd3_0130, EA_run3_0525_0006, 1W4F, 1URF, 5UCE, EEHEE_rd3_1615, HEEH_KT_rd6_0790, EEHEE_rd4_0005, 6SOW, EHEE_rd4_0877, 1E6H, HEEH_KT_rd6_3632, 2MW9, EHEE_rd1_0101, GG_run6_1310_0004, XX_run1_0461_0006, EEHEE_rd3_1049, r11_797_TrROS_Hall, 1PV0, GG_run4_0467_0002, EHEE_rd2_0191, 2LVN, EHEE_rd4_0172, EEHEE_rd3_1810, 2OCH, 1PGA, HHH_rd2_0181, 2BTT, v2_4UZX, XX_run8_1203_0001, r4_412_TrROS_Hall, 1A32, 1CSQ, r11_829_TrROS_Hall, EA_run7_1025_0001, 1F0M, EA_run2_0290_0001, HHH_rd4_0676, 2JN4</p>
Val and test	<p>GG_run6_0775_0006, HHH_rd4_0613, GG_run4_0284_0002, 2WXC, 2M7O, HEEH_KT_rd6_0793, r10_572_TrROS_Hall, r11_569_TrROS_Hall, 2LQK, 2K5P, 1UBQ, r18_3_TrROS_Hall, 2K5H, 1WCL, 2PTL, 2RU9, 1TUC, 1PSE, r14_263_TrROS_Hall, 1W4H, 1YEZ, HEEH_KT_rd6_1415, r11_1081_TrROS_Hall, v2_2LDM, 1GYZ, XX_run6_1020_0004, XX_run3_1384_0005, 2KWH, 2K28, 2KCF, 6ACV, HHH_rd4_0395, HHH_rd4_0124, 6EWT, 2OP7, XX_run6_1081_0004, EA_run3_1140_0005, 2LC2, EA_run6_0680_0006, 2MLB, 1QKH, 2K1B, 6XQC, 1QP2, 1I6C, 2KVS, 2KXD, 1SF0, GG_run6_0851_0003, 1V1C, HHH_rd1_0244, 3DKM, r12_757_TrROS_Hall, v2R31S_R32S_2N5D, 2M9I, 2L33, 2M0X, 2K9D, 2PFU, 2WNM, 2BTH, 2M9E, v2_1OGW, 1SIF, HHH_rd4_0557, v2_5XK5, v2_2LC2, 5LXJ, 2M9F, HEEH_KT_rd6_0746, 6EWU, r3_162_TrROS_Hall, 2YSF, EA_run3_0321_0005, 6EWS, r15_550_TrROS_Hall, HEEH_rd4_0094, 4C26, v2R14S_R16S_2L3X, HHH_rd1_0142, HHH_rd1_0949, 2MSG, GG_run5_1147_0004, 3ZGK, 1WR4, 5ZD0</p>