

Kinase domains with PDB structures with “ESCHERICHIA” contained within the EXPRESSION_SYSTEM field

Number of kinase domains returned: 136

Data for these kinase domains is listed at the end, sorted by target score.

Notes on selected kinases:

- **EGFR (TK) - 2 PDBs**
 - Both PDBs are false positives - only the substrate peptides were expressed in E coli
- **BRAF (TKL) - 3 PDBs**
 - PDBs:
 - 3C4C
 - Used an engineered form of BRAF, in which a number of solvent-exposed hydrophobic residues were mutated to more polar residues.
 - 4FK3
 - same article as above
 - 4JVG
 - different study, but looks like the same construct
- **JAK2 (TK) - 2 PDBs**
 - PDBs:
 - 2XA4
 - confirmed from article. BL21 cells. A few mutations.
 - 3ZMM
 - same group.
- **MET (TK) - 5 PDBs**
 - Example PDBs:
 - 2G15
 - 2006 paper - group at Plexxikon (Berkeley; corresponding author: Brian L West). They report yields > 1 mg/L for expression of Abl1, Src and Met kinases in E coli. They co-expressed with PTP1B tyrosine phosphatase. N-terminal His tag. Otherwise no modifications (WT sequences). Derived an XRC structure for Met kinase. Abl1 construct: G227-V515.
 - 3RHK
 - different group, followed Plexxicon protocol
- **MAPK14 (CMGC) - 187 PDBs**
 - (MK14_HUMAN below)
 - a P38 kinase
 - PDBs seem to comprise WT sequence
- **CDK2 (CMGC) - 191 PDBs**
 - No disease associations in UniProt entry, but other sources indicate association with smooth muscle tumor, oligodendroglioma, and Wikipedia mentions CDK2 inhibition as a possible strategy for prevention of chemotherapy-induced alopecia.

= List of PK domains with E coli expression host listed in PDB structure, ordered by priority score =

target_score = based on npubs, %mut, npk_pdb and ndisease_assocs (with strong penalty for pseudogenes and PK domains with unusually long or short sequences)
pk_length = aa length of PK domain
npubs = number of publications listed in PubMed
%mut = percentage mutations for this gene within all cBioPortal tumor sequencing data
npk_pdb = number of PDBs for which the PK domain is resolved
ndisease_assocs = from UniProt (not particularly reliable - working on integrating a more suitable resource)
nbioassays = from BindingDB

kinDB_id	target_score	family	pk_length	npubs	%mut	npk_pdb	ndisease_assocs	nbioassays	npdb w expr system	"*ESCHERICHIA*" & first 10 PDB codes
EGFR_HUMAN_P00533_PK0	100.0	TK	268	2948	4.954	59	1	6377	2 2RF9 4I21	
BRAF_HUMAN_P15056_PK0	74.8	TKL	261	986	7.055	28	8	901	3 3C4C 4FK3 4JVG	
JAK2_HUMAN_O60674_PK0	72.2	TK	276	999	1.971	31	6	1306	2 2XA4 3ZMM	
MET_HUMAN_P08581_PK0	70.2	TK	268	557	2.419	42	6	2319	5 2G15 3RHK 4EEV 4GG5 4GG7	
MK14_HUMAN_Q16539_PK0	69.1	CMGC	285	946	0.702	199	0	5224	187 1A9U 1BL6 1BL7 1BMK 1DI9 1IAN 1KV1 1KV2 1M7Q 1OUK	
VGFR2_HUMAN_P35968_PK0	68.2	TK	329	585	3.418	34	2	5526	3 1Y6A 1Y6B 2OH4	
CDK2_HUMAN_P24941_PK0	64.0	CMGC	283	563	0.690	337	0	3509	191 1BUH 1E9H 1F5Q 1FIN 1FQ1 1FVT 1FVV 1GY3 1H1P 1H1Q	
ABL1_HUMAN_P00519_PK0	62.4	TK	252	582	1.644	21	2	2746	6 2F4J 2G1T 2G2F 2G2H 2G2I 3UE4	
KIT_HUMAN_P10721_PK0	61.9	TK	349	682	2.595	6	4	1677	1 4HVS	
FGFR1_HUMAN_P11362_PK0	61.4	TK	290	306	1.794	15	7	1250	10 3C4F 3GQI 3GQL 3JS2 3KXX 3KY2 3RHX 4F63 4F64 4F65	
MK01_HUMAN_P28482_PK0	61.1	CMGC	289	1436	0.760	32	0	788	32 1PME 1TVO 1WZY 2OJG 2OJI 2OJJ 2Y9Q 3ISZ 3I60 3SA0	
INSR_HUMAN_P06213_PK0	60.2	TK	276	480	2.488	15	5	829	2 1RQQ 2AUH	
CHK2_HUMAN_O96017_PK0	57.9	CAMK	267	415	1.666	36	4	477	25 2CN5 2CN8 2W0J 2W7X 2WTC 2WTD 2WTI 2WTJ 2XBJ 2XK9	
FGFR2_HUMAN_P21802_PK0	57.6	TK	290	380	2.877	14	9	277	12 2PSQ 2PVF 2PVY 2PWL 2PY3 2PZ5 2PZP 2PZR 2Q0B 3B2T	
GSK3B_HUMAN_P49841_PK0	57.4	CMGC	285	722	1.323	42	0	2174	7 1J1B 1J1C 2JLD 2OSK 3MIS 3PUP 4DIT	
IGF1R_HUMAN_P08069_PK0	56.8	TK	276	611	2.025	16	1	1595	2 3LVP 3O23	
TGFR1_HUMAN_P36897_PK0	55.6	TKL	291	353	1.357	13	3	1074	1 1B6C	
CHK1_HUMAN_O14757_PK0	55.3	CAMK	257	321	1.266	104	0	2312	9 2E9N 2E9O 2E9P 2E9U 2E9V 2GHG 2YWP 3JVR 3JVS	
AURKA_HUMAN_O14965_PK0	53.0		251	384	0.823	66	0	1709	53 1OL5 1OL6 1OL7 2C6D 2C6E 2NP8 2W1C 2W1D 2W1E 2W1F	
MK08_HUMAN_P45983_PK0	52.2	CMGC	296	701	1.212	22	0	1190	22 1UKH 1UKI 2G01 2GMX 2H96 2NO3 2XRW 2XS0 3ELJ 3O17	
PLK1_HUMAN_P53350_PK0	51.5		253	391	1.648	12	1	1188	2 2V5Q 3THB	
MK10_HUMAN_P53779_PK0	51.1	CMGC	296	81	1.366	36	1	1310	36 1JNK 1PMN 1PMQ 1PMU 1PMV 2B1P 2EXC 2O0U 2O2U 2OK1	
MP2K1_HUMAN_Q02750_PK0	50.8	STE	294	277	1.427	29	1	790	14 1S9J 2P55 3DV3 3DY7 3E8N 3EQB 3MBL 3ORN 3OS3 3PP1	
FAK1_HUMAN_Q05397_PK0	50.2	TK	259	555	1.826	9	1	658	1 2IJM	
VGFR1_HUMAN_P17948_PK0	49.0	TK	332	430	3.150	1	2	1060	1 3HNG	
TIE2_HUMAN_Q02763_PK0	47.8	TK	273	179	2.230	6	2	749	3 2O08 2OSC 3L8P	
PI3K_HUMAN_P11309_PK0	47.6	CAMK	253	143	0.904	76	0	927	70 1XQZ 1XR1 1XWS 1YHS 1YI3 1YI4 1YVW 1YXS 1YXT 1YXU	
CSK21_HUMAN_P68400_PK0	47.5		286	544	1.196	38	0	442	38 1JWH 1NA7 1PJK 2PVR 2ZJW 3AMY 3AT2 3AT3 3AT4 3AXW	
ITK_HUMAN_Q08881_PK0	46.4	TK	253	79	1.999	16	1	766	5 1SM2 1SNU 1SNX 3QGW 3QGY	
HCK_HUMAN_P08631_PK0	46.3	TK	254	180	1.358	17	2	294	1 2HK5	
JAK3_HUMAN_P52333_PK0	45.4	TK	290	168	1.729	8	1	771	1 1YVJ	
BTX_HUMAN_Q06187_PK0	45.3	TK	254	212	1.849	12	2	256	1 1K2P	
KAPCA_HUMAN_P17612_PK0	45.2	AGC	255	448	1.041	19	0	592	15 2GU8 3AGL 3AGM 3AMA 3AMB 3NX8 3OOG 3OVV 3OWP 3OXT	
KSYK_HUMAN_P43405_PK0	44.9	TK	261	350	1.370	23	0	615	3 4DFL 4DFN 4F4P	
CDK9_HUMAN_P50750_PK0	44.4	CMGC	297	319	0.694	18	1	259	1 4IMY	
MAPK2_HUMAN_P49137_PK0	43.9	CAMK	262	104	1.097	22	0	1105	20 1KWP 1NXX 1NY3 2JBO 2JBP 2OZA 2P3G 2PZY 3A2C 3FFM	
PDPK1_HUMAN_O15530_PK0	43.5	AGC	261	164	0.654	47	0	509	1 2R7B	
AURKB_HUMAN_Q96GD4_PK0	43.1		251	254	0.752	1	1	1280	1 4AF3	
NTRK1_HUMAN_P04629_PK0	43.1	TK	272	245	2.121	3	2	331	1 4FOI	
KS6A3_HUMAN_P51812_PK1	43.0	AGC	258	128	1.413	5	2	375	5 4D9T 4D9U 4JG6 4JG7 4JG8	
JAK1_HUMAN_P23458_PK0	42.1	TK	279	254	2.167	12	0	634	2 3EYG 3EYH	
FAK2_HUMAN_Q14289_PK0	41.5	TK	259	243	1.573	10	1	227	2 3CC6 3ET7	
EPHA3_HUMAN_P29320_PK0	41.2	TK	262	52	3.952	21	1	164	21 2GSF 2Q02 2Q07 2Q09 2Q0B 2QOC 2QOD 2QOF 2QOI 2QOK	
ROCK1_HUMAN_Q13464_PK0	40.6	AGC	263	229	2.730	10	0	510	1 2V55	
MK03_HUMAN_P27361_PK0	39.8	CMGC	289	993	0.809	1	0	202	1 2ZQO	
DYR1A_HUMAN_Q13627_PK0	38.5	CMGC	321	108	1.745	5	1	270	5 2VX3 2W06 3ANQ 3ANR 4AZE	
KC1D_HUMAN_P48730_PK0	37.0	CKI	269	79	1.303	5	1	219	2 4HGT 4HNF	
DAPK1_HUMAN_P53355_PK0	36.9	CAMK	263	160	2.642	30	0	128	30 1IG1 1JKK 1JKL 1JKS 1JKT 1P4F 1WVW 1WVX 1WVY 2W4J	
CSKP_HUMAN_O14936_PK0	36.6	CAMK	265	81	1.748	8	2	72	8 3C0G 3C0H 3C0I 3MFR 3MFS 3MFT 3MFU 3TAC	
MK09_HUMAN_P45984_PK0	36.6	CMGC	296	183	1.187	2	0	772	2 3E7O 3NPC	
NEK2_HUMAN_P51955_PK0	36.6	NEK	264	78	0.967	20	0	252	20 2JAV 2W5A 2W5B 2W5H 2WQO 2XK3 2XK4 2XK6 2XK7 2XK8	
KPCT_HUMAN_Q04759_PK0	36.2	AGC	255	181	1.881	2	0	654	1 1XJD	
TTK_HUMAN_P33981_PK0	36.0		267	85	2.359	16	0	213	12 2ZMC 2ZMD 3CEK 3GFW 3H9F 3HMN 3HMO 3HMP 4BHZ 4BI0	
MERTK_HUMAN_Q12866_PK0	35.8	TK	272	81	2.006	4	1	176	4 2P0C 3BPR 3BRB 3TCP	
ACVR1_HUMAN_Q04771_PK0	35.2	TKL	295	92	1.309	6	1	125	1 3H9R	

[illegible]

OXSRL_HUMAN_Q95747_PK0	24.3	STE	275	33	0.948	2	0	79	2	2VWI	3DAK
VRK2_HUMAN_Q86Y07_PK0	22.5	CK1	291	29	1.109	1	0	72	1	2V62	
CDKL1_HUMAN_Q00532_PK0	22.3	CMGC	284	11	1.081	1	0	73	1	4AGU	
MARK3_HUMAN_P27448_PK0	22.2	CAMK	252	49	1.643	2	0	43	2	2QNJ	3FE3
HASP_HUMAN_Q8TF76_PK0	21.9		315	19	1.130	7	0	22	7	2VUV	2WB8 3DLZ 3E7V 3F2N 3FMD 3IQ7
MAPK3_HUMAN_Q16644_PK0	19.2	CAMK	261	37	0.649	4	0	17	4	3FHR	3FXW 3R1N 3SHE
KCC2A_HUMAN_Q9UQM7_PK0	14.8	CAMK	259	144	0.869	2	0	6	2	2VZ6	3SOA
ILK_HUMAN_Q13418_PK0	12.9	TKL	254	209	1.031	3	0	2	3	3KMU	3KMW 3REP
VRK1_HUMAN_Q99986_PK0	11.7	CK1	281	45	1.110	1	1	1	1	3OP5	
STRAA_HUMAN_Q7RTN6_PK0	9.5	STE	311	24	0.812	2	1	0	1	3GNI	
VRK3_HUMAN_Q8IV63_PK0	3.4	CK1	292	9	1.586	1	0	0	1	2JII	
E2AK3_HUMAN_Q9NZJ5_PK0	-3881.2		485	81	1.973	2	1	304	1	4G31	
CDC7_HUMAN_Q00311_PK0	-3885.0		517	64	1.179	4	0	316	1	4F99	
SRPK1_HUMAN_Q96SB4_PK0	-3889.4	CMGC	574	66	1.712	3	0	128	1	1WAK	
SRPK2_HUMAN_P78362_PK0	-3892.8	CMGC	604	37	1.358	1	0	117	1	2X7G	