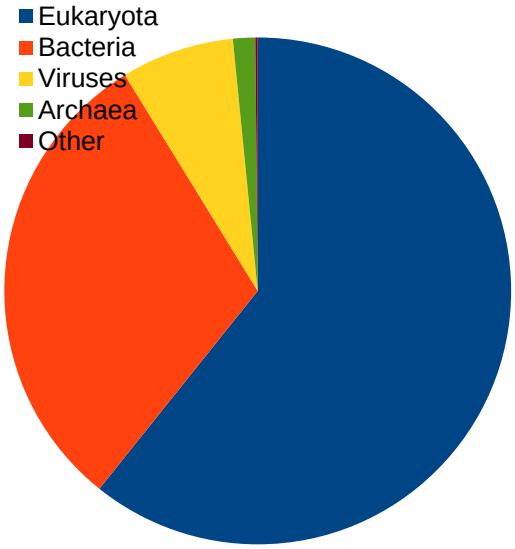
SM_File2: Taxonomic distribution of dataset



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SM_Figure 2.1: Pie-chart representing taxonomic distribution of protein structures used in DEELIG

Taxonomy and Species

Organism	**Number**
Homo sapiens	*1613*
Escherichia coli	*244*
Mycobacterium tuberculosis	*158*
Human immunodeficiency virus spp.	*152*
Bos taurus	*150*
Mus musculus	*139*
Rattus norvegicus	*94*
Saccharomyces cerevisiae	*64*
Pseudomonas aeruginosa	*53*
Bacillus subtilis	*48*
Escherichia virus T4	*40*
Pseudomonas putida	*34*
Streptomyces avidinii	*32*
Thermotoga maritime	*30*
Arabidopsis thaliana	*25*
Staphylococcus aureus	*25*
Oryctolagus cuniculus	*24*
Bacillus megaterium	*21*
Streptococcus pneumoniae	*19*
Lactococcus lactis	*18*
Hepacivirus C	*17*

Human immunodeficiency virus	*16*
Vibrio cholerae	*15*
Helicobacter pylori	*15*
Salmonella enterica	*15*
Gallus gallus	*14*
Lactobacillus casei	*13*
Vibrio harveyi	*13*
Eukaryota	*2400*
Bacteria	*1204*
Viruses	*285*
Archaea	*56*
Other	*6*

SM_Table 2.1: Taxonomic and species-specific distribution of protein structures used in training DEELIG

Domain Distribution

Domain Name	**Frequency**
p450	255
Pkinase	237
Carb_anhydrase	237
Pkinase_Tyr	201
Bromodomain	191
Hormone_recep	141
RVP	137
Neur_chan_LBD	134
Avidin	127
Ldh_1_N	92
Transthyretin	89
Lipocalin	88
PNP_UDP_1	81
HATPase_c	76
Gal-bind_lectin	68
Trypsin	68
VHL	68
rve	67
HSP70	65
DHquinase_II	56
NO_synthase	55
Lig_chan-Glu_bd	52
Pantoate_ligase	51
Phage_lysozyme	48

V-set	44
Glyco_hydro_1	44
FimH_man-bind	44
cNMP_binding	41
HPPK	39
SBP_bac_8	38
Asp	38
Aldo_ket_red	37
C1-set	35
SWIB	35
DAO	34
GST_C_3	34
adh_short_C2	34
DHFR_1	33
Ras	32
P-II	32
show	31
GST_N	31
PARP	30
TetR_N	29
P53	29
FabA	29
ketoacyl-synt	28
RdRP_3	28
SBP_bac_1	28
Flavodoxin_1	26
Aminotran_1_2	26
PA-IL	26
Aldedh	25
Jacalin	25
2OG-FeII_Oxy_3	24
PBP_GOBP	24
NNMT_PNMT_TEMT	24
Flavodoxin_2	24
YgbB	23
PH	23
DAHP_synth_1	23
tRNA-Thr_ED	23
EPSP_synthase	23
Thymidylat_synt	22
Pribosyltran	22
Flavin_Reduct	21
IF4E	21
GLF	21
FBPase	21

peroxidase	20
Pentaxin	20
SnoaL_2	20
Lactamase_B	19
FKBP_C	19
Dioxygenase_C	19
An_peroxidase	19
NDK	19
Hist_deacetyl	18
TMEM173	18
dUTPase	18
ECH_1	18
AMPK1_CBM	18
Glyco_hydro_18	18
Aminotran_3	18
Filo_VP35	18
Peptidase_M10	18
LysR_substrate	17
PDEase_I	17
Peripla_BP_4	17
BCDHK_Adom3	17
PALP	17
Nitroreductase	17
DXP_reductoisom	16
BPL_C	16
DIOX_N	16
HMG-CoA_red	16
Thiolase_N	16
Pyr_redox_2	16
NTP_transferase	16
E1-E2_ATPase	16
4HBT	16
F420H2_quin_red	15
RbsD_FucU	15
NAD_binding_1	15
Pterin_bind	15
Sugar-bind	15
Oxidored_FMN	15
Phospholip_A2_1	15
S_100	15
Peripla_BP_2	15
Arginase	14
DctP	14
polyprenyl_synt	14
Acetyltransf_3	14

SET	14
Iso_dh	14
ABC_tran	14
SBP_bac_3	13
FAD_binding_3	13
Y_phosphatase	13
Peptidase_M4_C	13
LRR_8	13
Globin	12
COesterase	12
ArgoMid	12
Pan_kinase	12
CBS	12
NUDIX	11
DSBA	11
Enterotoxin_b	11
GP120	11
Thy1	11
Putative_PNPOx	11
Glyco_hydro_20	11
2-Hacid_dh_C	11
DHO_dh	11
ADH_zinc_N	11
Trp_syntA	11
NAGidase	11
Amidase_2	11
GTP_EFTU	11
Phosphorylase	11
Macro	11
Glyco_transf_6	11
Thymidylate_kin	10
Synapsin_C	10
Choline_kinase	10
NAPRTase	10
HpcH_HpaI	10
Exotox-A_cataly	10
FeoB_N	10
Redoxin	10
Pep_deformylase	10
Adenine_glyco	10
Antibiotic_NAT	10
CTP_transf_like	10
AlaDh_PNT_C	10
TPP_enzyme_N	10
Thia_YuaJ	10

Usp	10
Mab-21	10
PHZA_PHZB	10
MoaC	9
Rad51	9
PGK	9
Fungal_lectin	9
JmjC	9
Ribonuclease	9
Peptidase_M1	9
Serum_albumin	9
Orn_Arg_deC_N	8
SQS_PSY	8
Cytochrome_B	8
Ferritin	8
OmpA	8
ILEI	8
TGT	8
GDP_Man_Dehyd	8
Semialdhyde_dhC	8
RnaseA	8
Amino_oxidase	8
CPSase_L_D2	8
adh_short	8
7tm_1	8
Bcl-2	8
Rep-A_N	8
PFK	8
F_bP_aldolase	8
OTCace_N	8
Alpha_L_fucos	8
CoA_transf_3	8
Adeno_knob	8
Citrate_synt	8
GMP_PDE_delta	8
HTH_Crp_2	8
SBP_bac_5	8
WD40	8
Flu_PB2	8
LigT_PEase	8
EF-hand_1	7
Gag_p24	7
Ricin_B_lectin	7
PilZ	7
ADPrib_exo_Tox	7

Laminin_G_1	7
Abhydrolase_6	7
Bet_v_1	7
Peptidase_C14	7
Prenyltransf	7
PAS_3	7
Lectin_legB	7
Pro_isomerase	7
AMP-binding	7
RicinB_lectin_2	7
APH	7
Polyketide_cyc2	7
PrmA	7
Sec7	7
Peptidase_C1	7
MIF	7
SBP_bac_6	7
F5_F8_type_C	7
Glyco_hydro_7	7
PdxJ	6
Xlink	6
Hydrolase	6
Cu-oxidase	6
DHquinase_I	6
Hyd_WA	6
MHC_I_3	6
Rotamase	6
Alpha_kinase	6
AA_kinase	6
Septin	6
SBP_bac_11	6
AIRC	6
ADH_N	6
Glyco_hydro_47	6
Rubis-subs-bind	6
VWA	6
Serpin	6
DapB_C	6
Peripla_BP_1	6
cobW	6
Abhydrolase_3	6
Peptidase_M17	6
PfkB	6
Chromo	6
Arm	6

SusD_RagB	6
QRPTase_C	5
Lectin_C	5
OKR_DC_1	5
EAL	5
Flavoprotein	5
MeaB	5
AAA	5
PI3Ka	5
His_binding	5
AAA_26	5
ApbA_C	5
DMRL_synthase	5
Me-amine-dh_L	5
BTB	5
Tubulin	5
CRAL_TRIO	5
tRNA-synt_1	5
Glyoxalase	5
Nitrophorin	4
Peptidase_C80	4
Tyrosinase	4
Neur	4
Autoind_bind	4
NAD_synthase	4
OpuAC	4
Flavi_NS5	4
HTH_27	4
Auxin_BP	4
TFR_dimer	4
Chorismate_synt	4
Enoyl_reductase	4
CIMR	4
rhaM	4
PAF-AH_p_II	4
O-FucT	4
Hfq	4
Spermine_synth	4
RNase_H	4
WWE	4
UDPG_MGDP_dh_N	4
ACPS	4
PARP_regulatory	4
Spin-Ssty	4
03/DD/YY	4

DPPIV_N	4
SIR2	4
DOT1	4
FAD_binding_4	4
GBP	4
MBT	4
TIM	4
Glyco_transf_41	4
Methyltransf_4	4
RdRP_1	4
CoA_binding_2	4
DNA_pol3_beta_2	4
Abhydrolase_2	4
DHH	4
Kringle	4
Piwi	4
UbiA	4
tRNA-synt_2	4
tRNA-synt_1b	4
CBM_48	4
Amidinotransf	4
DAHP_synth_2	4
AraC_binding	4
Pept_tRNA_hydro	4
L_protein_N	4
UPRTase	4
RIP	4
TrkA_N	4
Peripla_BP_3	4
Methyltransf_3	4
Alk_phosphatase	4
Methyltransf_25	4
FMN_dh	4
Glycos_transf_2	4
OCD_Mu_crystall	4
IU_nuc_hydro	4
ATP-grasp	4
Peptidase_S29	4
CdAMP_rec	4
RuBisCO_large	4
NMT	3
Hexokinase_2	3
LamB	3
MMR_HSR1	3
OS-D	3

Ribonuc_L-PSP	3
FAD_binding_7	3
MarR	3
OTCace	3
DNA_ligase_aden	3
PadR	3
SHMT	3
RIO1	3
BPL_LplA_LipB	3
LpxC	3
Alpha-amyl_C2	3
Ribonuc_red_lgC	3
Bac_luciferase	3
APS_kinase	3
FtsJ	3
Sulfotransfer_1	3
Acetyltransf_14	3
PanZ	3
EIIC-GAT	3
Bmp	3
Folate_rec	3
TetR_C_1	3
HAD_2	3
IIGP	3
Lipocalin_7	3
TetR_C_24	3
Metalloenzyme	3
2-oxoacid_dh	3
AnmK	3
Prenyltrans	3
BNR_2	3
AIG1	3
BioY	3
Dynamin_N	2
IL2	2
HD	2
YBD	2
Guanylate_cyc	2
PI-PLC-X	2
S-methyl_trans	2
IlvN	2
Gp_dh_C	2
Kinesin	2
HIT	2
DHDPS	2

Ubie_methyltran	2
WH1	2
Dak1	2
Glucodextran_N	2
Glyco_hydro_76	2
CYTH	2
Glyco_hydro_14	2
Reprolysin_5	2
Sigma54_activat	2
ParA	2
Me-amine-dh_H	2
Methyltransf_33	2
NeuB	2
NAGLU	2
CoA_binding	2
Transferrin	2
HBM	2
HSP90	2
CM_2	2
ACP_syn_III_C	2
Epimerase	2
Sial-lect-inser	2
Amidase	2
Myosin_head	2
MHC_I	2
Glyco_hydro_3	2
PAP_assoc	2
ROK	2
YcgR_2	2
NAD_binding_4	2
AICARFT_IMPCHas	2
MoeA_N	2
TNF	2
Lipocalin_2	2
PAS_4	2
RasGEF	2
SpoU_methylase	2
Mur_ligase_M	2
ADK	2
DcpS	2
TctC	2
SNF	2
Trehalase	2
CBM_6	2
ATP-synt_ab	2

Ald_Xan_dh_C2	2
Arf	2
Nucleos_tra2_C	2
3HCDH_N	2
NEAT	2
Actin	2
Peripla_BP_6	2
Aldose_epim	2
G-alpha	2
Lon_C	2
Methyltransf_2	2
Glycolytic	2
ZipA_C	2
Pneumo_ncap	2
NMT1	2
Beta-lactamase2	2
Oxysterol_BP	2
HipA_C	2
SKI	2
Asp_Glu_race	2
Peptidase_S21	2
Fic	2
LON_substr_bdg	2
6PF2K	2
Leukocidin	2
PhzC-PhzF	2
GST_C_2	2
UTRA	2
CVNH	2
Glyco_hydro_43	2
GGDEF	2
ATP-gua_Ptrans	2
Diphtheria_C	2
PilM_2	2
Fusion_gly	2
Abhydrolase_1	2
HI0933_like	2
6PGD	2
Carboxyl_trans	2
Glyco_hydro_15	2
FGGY_N	2
Cupin_5	2
VP4_haemagglut	2
NmrA	2
XylR_N	2

tRNA_m1G_MT	2
PGM_PMM_I	2
tRNA-synt_1g	2
Glucosamine_iso	2
Fumble	2
ATP-synt_DE_N	2
HN	2
FYVE	2
dCache_1	2
HMGL-like	2
Mannosidase_ig	2
TPP_enzyme_M_2	2
IGPS	2
GMC_oxred_N	2
Peptidase_C10	2
MDD_C	2
PRMT5_TIM	1
NAD_kinase	1
Phosphonate-bd	1
PX	1
Aminotran_4	1
Sua5_yciO_yrdC	1
Ferrochelatase	1
PBP_like_2	1
Glyco_hydro2_C5	1
SGL	1
Transketolase_N	1
FAD_binding_2	1
Regulator_TrmB	1
PEPCK_GTP	1
PH_9	1
BioW	1
Glyco_hydro_85	1
Peptidase_M27	1
Pirin_C	1
DNA_topoisoIV	1
Inhibitor_I9	1
RVT_connect	1
FAD_binding_6	1
Scytalone_dh	1
JHD	1
Calici_coat_C	1
Autoind_synth	1
DEAD	1
PH_12	1

Pro_dh	1
N6_N4_Mtase	1
PAE	1
Amidohydro_1	1
Clp_N	1
ABC_ATPase	1
Isochorismatase	1
PI3_PI4_kinase	1
7tm_2	1
Peroxidase_2	1
DrrA_P4M	1
EF-hand_7	1
DUF5115	1
FBPase_3	1
HRM	1
ACBP	1
TcdA_TcdB	1
CAT	1
Arabino_trans_C	1
IMPDH	1
FmrO	1
Tachylectin	1
HisG	1
Glyco_trans_1_4	1
Peptidase_C3	1
Kelch_1	1
KIX	1
53-BP1_Tudor	1
SusF_SusE	1
TP_methylase	1
DNA_gyraseB	1
OMPdecase	1
AKAP7_NLS	1
2OG-FeII_Oxy_2	1
Chal_sti_synt_N	1
GDI	1
PARG_cat	1
CAP	1
NTF2	1
UDPGP	1
Neocarzinostat	1
GHMP_kinases_C	1
SRPRB	1
ENTH	1
Exotox-A_bind	1

Transpeptidase	1
DUF1080	1
4HBT_2	1
HhH-GPD	1
DNA_pol3_delta2	1
His_Phos_2	1
MFS_1	1
PPV_E2_N	1
Menin	1
DAGK_cat	1
MIR	1
Ins_P5_2-kin	1
His_biosynth	1
RabGAP-TBC	1
SPRY	1
DUF4154	1
C2	1
Hexapep	1
PHD	1
Glycos_transf_1	1
Carb_kinase	1
FTO_NTD	1
RsgA_GTPase	1
PNTB	1
Triabin	1
AAA_lid_9	1
GTP1_OBG	1
DUF3372	1
UQ_con	1
YCII	1
Haspin_kinase	1
T3SS_TC	1
HsbA	1
MaoC_dehydrat_N	1

SM_Table 2.2: Frequency of domain distribution of protein structures used for training DEELIG

Domain Distribution in dataset

Set	Total	p450	pkinase	pkinase_tyr
Training	6539	251	233	195
Validation	498	24	20	13
Test	199	2	6	8

SM_Table 2.3: Distribution of kinases in our dataset