

Supplementary Table 1. Ramachandran plot parameters for the models built. Sum may differ from 100% due to truncation error.

Name	length	1UV5					1Q41				
		Core	Allowed	Generously allowed	Disallowed	z-score	Core	Allowed	Generously allowed	Disallowed	z-score
HsGSK-3 β	292	84.1%	13.9%	0.0%	2.0%	-11.07	86.5%	12.5%	0.3%	0.7%	-11.11
RmGSK-3	285	91.3%	6.3%	1.2%	1.2%	-10.35	92.1%	6.7%	0.4%	0.8%	-10.47
AaGSK-3	285	90.4%	7.6%	0.8%	1.2%	-10.03	90.4%	8.4%	0.4%	0.8%	-10.05
SHAGGY	285	91.7%	6.3%	0.8%	1.2%	-9.48	90.9%	7.9%	0.4%	0.8%	-9.58
BmGSK-3	277	88.8%	9.2%	1.7%	0.4%	-9.21	89.6%	8.8%	1.7%	0.0%	-9.01
SmGSK-3	285	89.3%	8.3%	0.8%	1.6%	-9.68	92.1%	6.7%	0.4%	0.8%	-9.43
AdGSK-3	284	89.6%	8.0%	0.8%	1.6%	-9.7	89.6%	8.8%	0.4%	1.2%	-9.58
PbrGSK-3	284	88.8%	8.8%	0.8%	1.6%	-9.53	90.8%	8.0%	0.4%	0.8%	-9.51
AtGSK-3	268	89.4%	7.6%	1.3%	1.7%	-8.75	89.8%	8.9%	0.4%	0.8%	-8.74
AfGSK-3	284	89.6%	7.6%	1.2%	1.6%	-9.37	89.2%	9.2%	0.8%	0.8%	-9.36
CgGSK-3	284	88.8%	9.2%	0.8%	1.2%	-9.31	90.0%	8.8%	0.4%	0.8%	-9.29
CnGSK-3	332	89.3%	8.3%	1.7%	0.7%	-9.65	91.0%	8.0%	0.3%	0.7%	-9.4
CdGSK-3	283	89.1%	8.5%	0.8%	1.6%	-9.74	89.1%	10.1%	0.0%	0.8%	-9.37
CiGSK-3	284	88.4%	8.8%	1.2%	1.6%	-10.01	90.0%	8.4%	0.8%	0.8%	-9.67
PfGSK-3	287	90.7%	7.8%	0.0%	1.6%	-9.69	89.9%	8.9%	0.4%	0.8%	-10.02
PbGSK-3	287	89.9%	7.8%	0.8%	1.6%	-9.59	89.1%	9.3%	0.4%	1.2%	-9.84
LiGSK-3	330	87.3%	10.3%	1.0%	1.4%	-8.55	89.3%	9.3%	0.7%	0.7%	-7.97
LmGSK-3	330	87.6%	9.3%	1.4%	1.7%	-8.36	87.2%	11.0%	0.7%	1.0%	-8.27
LdGSK-3	330	87.3%	10.3%	1.0%	1.4%	-8.55	86.9%	10.7%	0.7%	1.7%	-7.87
LmxGSK-3	330	87.6%	10.0%	1.0%	1.4%	-8.13	87.3%	10.7%	1.0%	1.0%	-7.94
LbGSK-3	327	87.4%	9.4%	1.4%	1.7%	-8.15	90.2%	8.7%	0.3%	0.7%	-8.01
TbGSK-3	327	89.5%	8.8%	0.4%	1.4%	-8.92	88.4%	10.5%	0.7%	0.4%	-8.12
TPK3	298	89.1%	8.7%	1.1%	1.1%	-9.25	90.9%	7.9%	0.4%	0.8%	-8.95

Supplementary Figure 1. The phylogenetic tree of the kinases studied.

