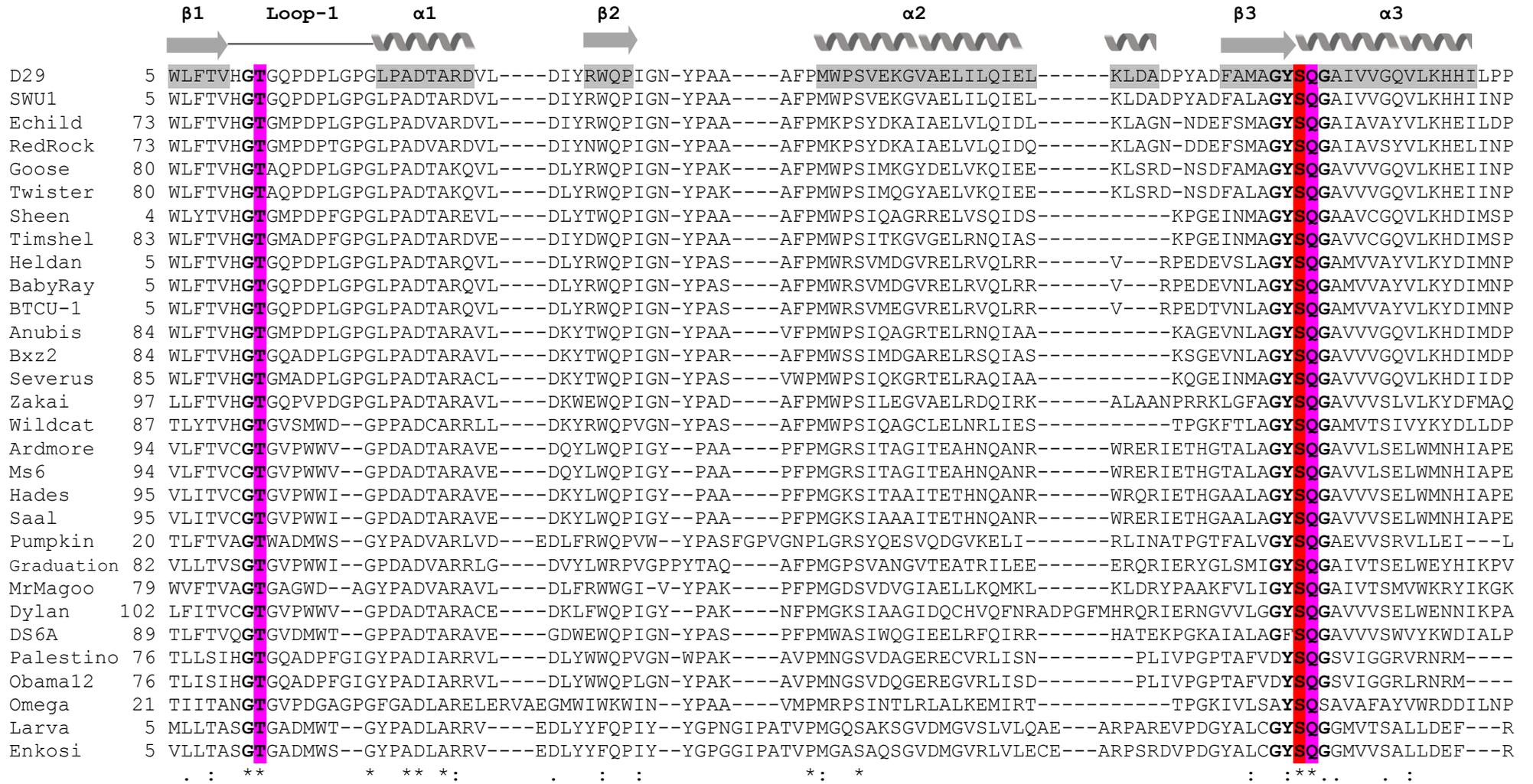


a

Region-1

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D29 1 -----M-----SKP
SWU1 1 -----M-----SKP
Echild 1 MSLQLG-----SNGDLVNRWIRVMKARFASYA-----GKLRED----AYFGLDDQAVQREYETRTHQ-----TPDGIVTDGDLAY--LLP-----AKP
RedRock 1 MSLKVG-----SSGEVVSRWIRVMKARFVSYA-----GKLAVD----GYFGLDDAEVQREYERRTGQ-----TPDGIVTDGDLAY--LLP-----RKP
Goose 1 MALKVG-----SSGPLVNAWIRTMNARFESYSKAYDGGPLRED----AYFGYDDAEVQREYERRTGQ-----PVDGEVSDHDLVALGLIT-----EKP
Twister 1 MPLKLG-----SSGELVNAWIRTMNSRFESYSKAYDGGPLRED----AYFGYDDAEVQREYERRTGQ-----PVDGEVSDHDLVALGLIT-----EKP
Sheen 1 -----MTR
Timshel 1 MILKVG-----STGQVVDWQAEMLERYPYAKAADGGPLKVD----GYFGYDDEAVQVEYEFRTGQ-----PIDREVSQGDLDYLGIKTDS---FKGR
Heldan 1 -----MSDR
BabyRay 1 -----MSDR
BTCU-1 1 -----MSDR
Anubis 1 MPLRVGSND-----ANTGGLVSRWQKTMRLARFQAYAKAYDGGPLRVD----GYFGYDDADVQREYERRTHQ-----TVDGEVSDADLRALGLEA-----AKR
Bxz2 1 MPLRVGSND-----ANTGGLVSRWQKTMRLARYAAYAKAYDGGPLRVD----GYFGYDDADVQREYERRTHQ-----VVDGEVSDADLRALGLEA-----AKR
Severus 1 MPLRLG-----DRNDTVREWRYIMSKRFSGYARALGPLPT-DT----NEFGPRAKSWQEEYERRTGQ-----PVDGEVSDLDLDFALGVSVSPHAPGPTR
Zakai 1 --MAVGPDKWIGYGLGDSGIPVLTARQKLKAKF-SYAKH-----LRET----TLYDNE LLPVLIEYQLRKNVEFAKAGKKLLRTDGI LDYATQVAIGVVI--PVALVKP
Wildcat 1 ----MRVAGQWVGWGLGDIDPKVQDMKRFLKRKF-SYARES-----LDDS----EYDEMTMRVVMQMANY-----GDL DITGVMNYATQVRSGLKVEK--PPLP
Ardmore 1 ----MRIDGQYVGLGPGDRSDEIRKIKAFMRRKF-SYAATLA---DT-----EFYDEAMTAVVAEMQSRynt--AGHLRDGLYIPGIINAETKYVMGYLSRPV-IDTRP
Ms6 1 ----MRIDGQYVGLGPGDSSEEIRRIKTFMRRKFASYAGDLA---DT-----PLYDEQMTAAVAEMQARYNT--AGQLRDGLYIPGIINAETKYVMGYLSRPV-IDTRP
Hades 1 ----MRIDGQYVGLGPGDSSEEIRRIKTFMRRKFASYAGDLA---DT-----PLYDEQMTAAVAEMQARYNT--AGQLRDGLYIPGIINAETKYVMGYLSRPV-IDTRP
Saal 1 ----MRIDGQYVGLGPGDSSEEIRRIKTFMRRKFASYAGDLA---DT-----PLYDEQMTAAVAEMQARYNT--AGQLRDGLYIPGIINAETKYVMGYLSRPV-IDTRP
Pumpkin 1 -----MTTYGELKALRLG----VKYVRH
Graduation 1 -----MPLKLGDRNPTVRRWREVMARFAGYARVHGPLPTDTDEFGP-----RAEAWQTEYE-----SRTFQPLDGIVSDDD---LRALGIPAPEDTRP
MrMagoo 1 -----MAWIGWQEGMEGLPVLA AIGELRAKF-SYGKQ-----LELT----QKFTPELTQAIKTFQVKKG-----GLRTDGLVLDYATQAALGVPE-----ALKP
Dylan 1 ----MRIGGEYVGLGLGDASEEIGRIRDFMRRKFRSYAGNLP---DTRNALGLPLFDEPMTVAVTEMQGRYLQ--SGELRDGLFIFGIINAETKYVMGYLERPPGPDTRP
DS6A 1 -----MTWIGWQQGMAGEPVAAAKRELRRKF-SYAKH-----LDDS----DVFDELLAVLIEYQQKKNAT---GYTPRLREDGVL DWATQVAIGTVQTGP-PPKAG
Palestino 1 -----MLKLGSSGLMVSAAWTAVMRLRFASYALGVNGQPIKVD----GYFGYDEEKVQKEYQLRTGQ-----FPSGQVSREDLHRLGLLP-----
Obama12 1 -----MLKLGSNGLMVAAWTAVMIRIRFASYALGVNGLPIKVD----GYFGYDEEKVQKEYQRRTGQ-----FPSGQVSREDLHRLGLLP-----
Omega 1 -----MSLWPEIR---AMLNGEFYVPAG
Larva 1 -----MSKP
Enkosi 1 -----MSKP
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b



c

		$\alpha 4$	$\beta 4$	Loop-2	$\alpha 5$	$\beta 5$	Loop-3	$\alpha 6$	L-4	$\alpha 7$	$\alpha 8$				
D29	100	TGRLHRE	--LHRLKKVIFW	GNP	MRQKGF	AHSDEWIHPVAAPDTL	----	GILE-DRLENLE	----	QYGF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYEVA
SWU1	100	RGRLHRE	--LHRLRKVIFW	GNP	MRQKGF	AHTDEWIHPVAASDTM	----	GILE-DRLENLE	----	QYSF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYEVA
Echild	167	KGRLHKY	--VNRLKKVVMW	GNP	MRQKGF	AHFDEWIHPVAAPDTM	----	GILE-DRLENLEQA	----	MQYGF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYEVA
RedRock	167	KGRLHKY	--VHRLKKVVLW	GNP	MRQKGF	AHFDEWIHPVAGPDTM	----	GILE-DRLEALEQA	----	MKVYGF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYEVA
Goose	168	KGRLHKY	--LHRLKKVVFVW	GNP	MRQKGI	AHFDEWIHPVAGPDTM	----	GILE-DRLENLE	----	QYDF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYQVA
Twister	168	NGRLHKF	--LHRLKKVVFVW	GNP	MRQKGI	AHFDEWIHPVAGPDTM	----	GILE-DRLENLE	----	QYDF	EVDRDYAHD	----	GDMYASIKED	----	DMHEYQVA
Sheen	94	TGRLHHR	--LGDVRKVVFW	GNP	MRQQGI	AHSDEWVHPVASPDTM	----	GILE-DRLEGLE	----	NAPF	EVDRDYAHQ	----	GDMYASIKAD	----	DMHEYQVA
Timshel	173	SGSLHHR	--LKDVRKVVFW	GNP	MRQQGI	AHTDEWIHPVASPDTM	----	GILE-DRLEGLE	----	DAPF	EVDRDYAHE	----	GDMYASIKAD	----	DMHEYEVA
Heldan	97	AGEFHYL	--LHQVRKVVFW	GNP	MRQGI	AHDDRWIHRIAAPDTH	----	GIME-DRLEGLE	----	HAPF	EVDRDYAHD	----	EDMYASIRDD	----	DMHEYQIA
BabyRay	97	AGEFHYL	--LHQVRKVVFW	GNP	MRQQGI	AHDDRWIHRIAAPDTH	----	GIME-DRLEGLE	----	HAPF	EVDRDYAHD	----	EDMYTSIRDD	----	DMHEYQIA
BTCU-1	97	AGEFHYL	--LHQVRKVVFW	GNP	MRQGI	AHDDRWIHRIAAPDTH	----	GIME-DRLEGLE	----	HAPF	EVDRDYAHD	----	EDMYASIRDD	----	DMHEYQIA
Anubis	174	KGSLHHR	--LGDVRKVVVMW	GNP	MRQKGI	AHDDRWIHKVAGPDTY	----	GILE-DRLEGLD	----	KAPF	EVDRDYAHE	----	DDMFASVRDD	----	DIHEYQIA
Bxz2	174	KGSLHHR	--LGDVRKVVVLW	GNP	MRQGI	AHFDEWIHPVAGPDSY	----	GILD-DRLEGLE	----	KAPF	EIRDYAHA	----	GDMYASITDG	----	DKDEYKIA
Severus	175	AGPLHHR	--LGDVRKVVFW	GNP	MRQQGI	QHDDQWIHEIAPADTH	----	GILTFDLLEGLE	----	RFPHI	QVRDYAHK	----	GDMYACNTDD	----	QAAEYKRA
Zakai	192	GGEFHDQYEAGQVLA	VVTW	GNP	MRE	RGVQHGDGWKE-TAPADTE	----	GILE-DRLEGTP	----	AFWRE	YAHK	----	GDMYAACELTG	----	VQRGDNKRA
Wildcat	175	MGR LHHR	--LPDFMGGVTW	GNP	MRE	MKGAWTDGV-GAVAGQNG	----	GIAE-DRLVGTP	----	WNWR	DYAHK	----	GDLYTDCEFD	----	DEGEYKRS
Ardmore	186	DGSLRWM	--KPHVRKAVTW	GNP	NREL	GHVWADHGGSPMAPSNTQ	----	GVSS-N	----	G-MRNT	PDWWRDYAHQ	----	GDLYACTEPG	----	DTQEV RNA
Ms6	186	DGSLRWM	--KPHVRKAVTW	GNP	NREL	GHVWADHGGSPMAPSNTQ	----	GVSS-N	----	G-MRNT	PDWWRDYAHQ	----	GDLYACTEPG	----	DTQEV RNA
Hades	187	TGSLHWM	--KPHIEKAVTW	GNP	NREL	GHVWADHGGSPMAPSNTQ	----	GVSS-N	----	G-MRDT	PPWWRDYAHQ	----	GDLYACTEPG	----	DTQEV RNA
Saal	187	DGSLHWM	--KPHIEKAVTW	GNP	NREL	GHVWADHGGSPRAPSNTO	----	GVSS-N	----	G-MRDT	PPWWRDYAHQ	----	GDLYACTEPG	----	KSGEIITS
Pumpkin	113	FGSLRHR	--LKDFIGGGCF	GNP	YRAK	GVSYPGSSL-PTSGH	----	GIAP-VNLAPDI	----	LPAEM	WEEWNE	----	GDLYAQNLDG	----	DSGEMKTA
Graduation	176	TGRLHWV	--KDHVRGAVTF	GNP	MRET	GKVPNPGGQL-PSAKSH	----	GIAD-Q	----	L-MVD	TPDWRNYAHK	----	GDLYTDCE-G	----	DSGEMKTA
MrMagoo	173	--DL	-----EKRIIGSITF	GNP	CRE	LGAVANGVAE-GIPIPEGR	----	GIGD-DRLQSTP	----	EWYD	FAHGANS PFGRDIYTDTPDD	----	DTGEMMTA	----	
Dylan	200	NGSLHWA	--KDYVVKAVTW	GNP	NRE	VGAVWPDYGGSPMASLTSQ	----	GVSS-T	----	G-MRDT	PSWWRNYAHA	----	GDLYAAAEPG	----	DSQQDKNA
DS6A	182	GGMLHDL	--LPQVAAGVTW	GNP	MAEK	GKFGHGNRFAG-WPVPAGM	----	GINR-DRLENTP	----	ALWLD	FGHGRNSPWGQDIYCDRPN	----	LAGQDMEL	----	
Palestino	169	----RRKELRGELVAAA	SF	GNP	MRLR	GHYAGNVD-----PGGE	----	GIDPRQELAAE	----	PFR	VELAAK	----	GDLYTTCPGG	----	QSGEMERA
Obama12	165	----RRKELRGELVAAA	SF	GNP	MRLR	GHYAGNVD-----PGGE	----	GIDPRQELAAE	----	PFRI	ELAAK	----	GDLYTTCPGG	----	QSGEMERA
Omega	110	DGELHDR	--LDDIVAVILY	GNP	VRAP	GIAYGNELGGQSAPGKLNHVTGGIAGPDCLRPEECVHPVTGRRI	----	GINR-DRLENTP	----	ALWLD	FGHGRNSPWGQDIYCDRPN	----	LAGQDMEL	----	
Larva	101	TGRLKSV	--GHKLMAGSTF	GNP	WRE	LAD-----GGR	----	GISD-RRI	----	A	-----GTPDFWVDEFDP	----	GDIYANVPNN	----	DVGADMTA
Enkosi	101	TGRLRHL	--NGKLMAGSTF	GNP	WRE	LDSN-----GGR	----	GISD-RRI	----	V	-----GTPDFWVDEFDP	----	GDIYANVPNN	----	DVGDDMTA
				***				*	:				*::		

d

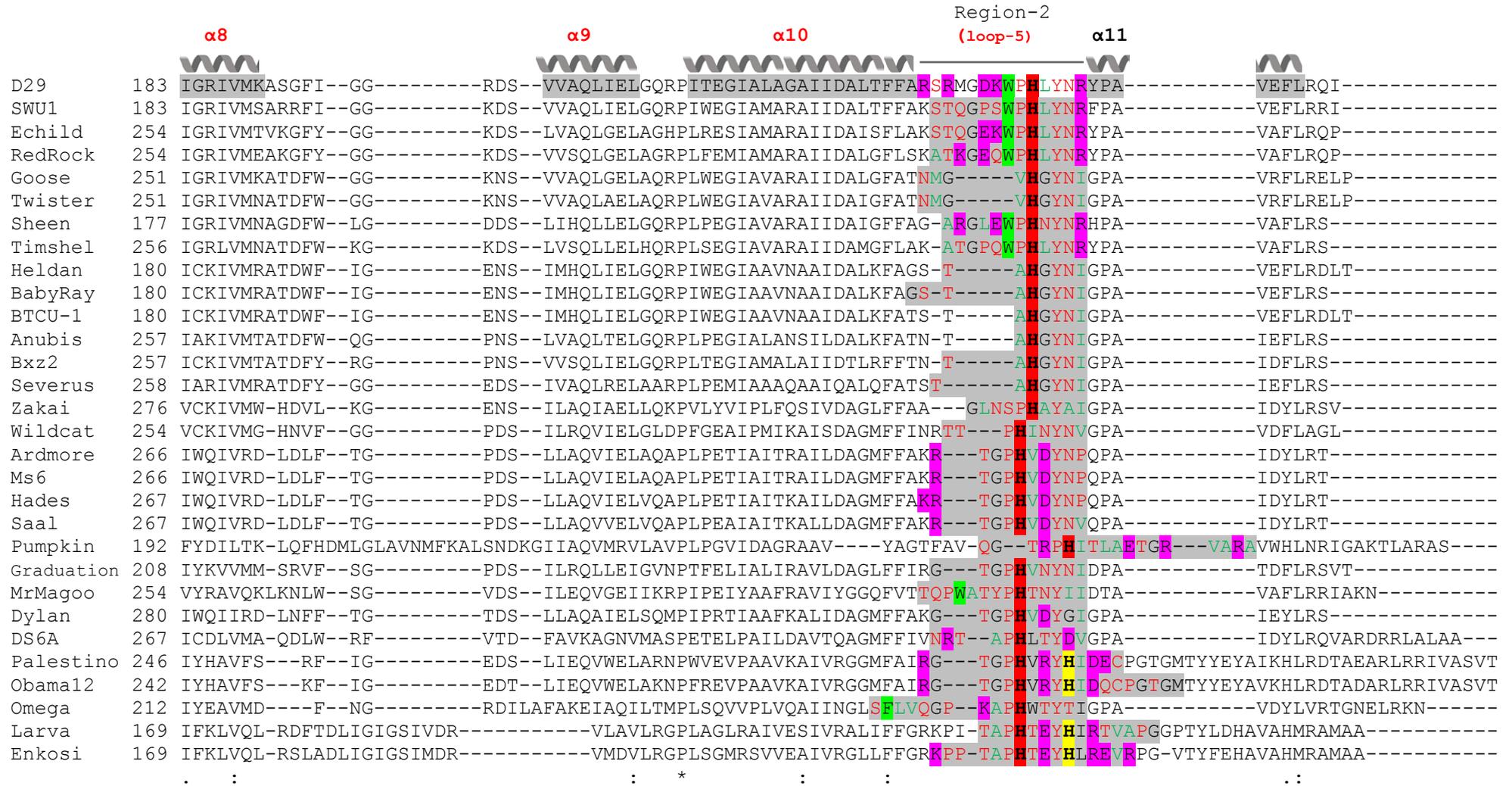


Figure S3: Multiple sequence alignment of LysB-D29 with its homologous lysB proteins. Identical residues are labeled by Asterisk, conserved residues labeled by colon and full stop indicates semi-conserved residues. Residues forming the active site are shaded in red color. Extra His residues are highlighted in yellow color. Oxyanion hole and GXP residues are shaded in pink. Residues forming β -strands and α -helices are highlighted in gray. Region-1 constitutes extra N-terminal residues. Region-2 constitutes residues forming hypervariable loop-5. Loops, β -strands and α -helices forming linker domain are in red. Residues forming loop-5 in each LysB model are highlighted in gray. Polar non-charged residues are in red, polar charged residues are highlighted in pink. Non-polar aliphatic residues are in green, non-polar aromatic residues are highlighted in green.