Supplementary Information for:

Structural basis of PAM recognition and target DNA unwinding by the CRISPR-associated endonuclease Cas9

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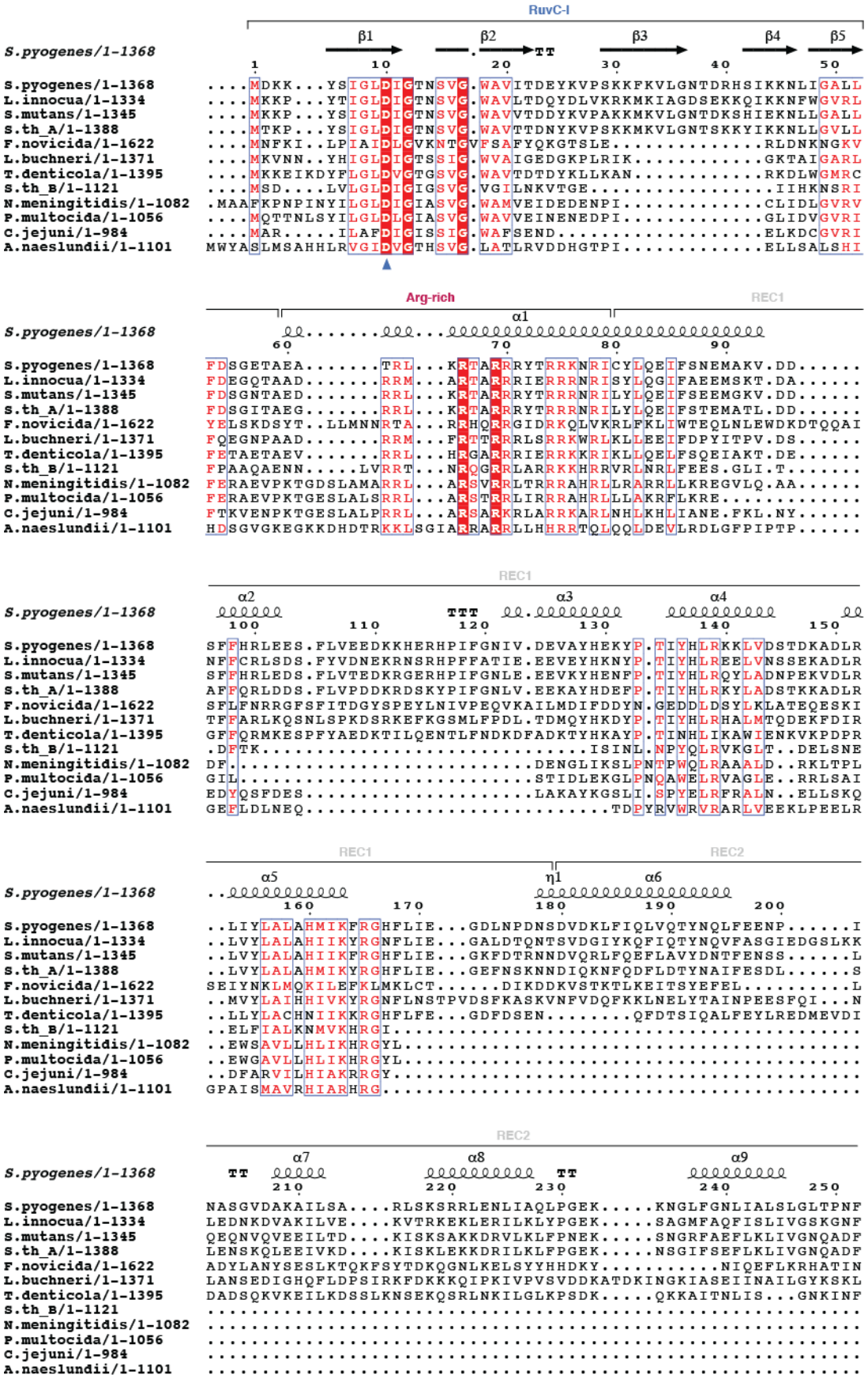
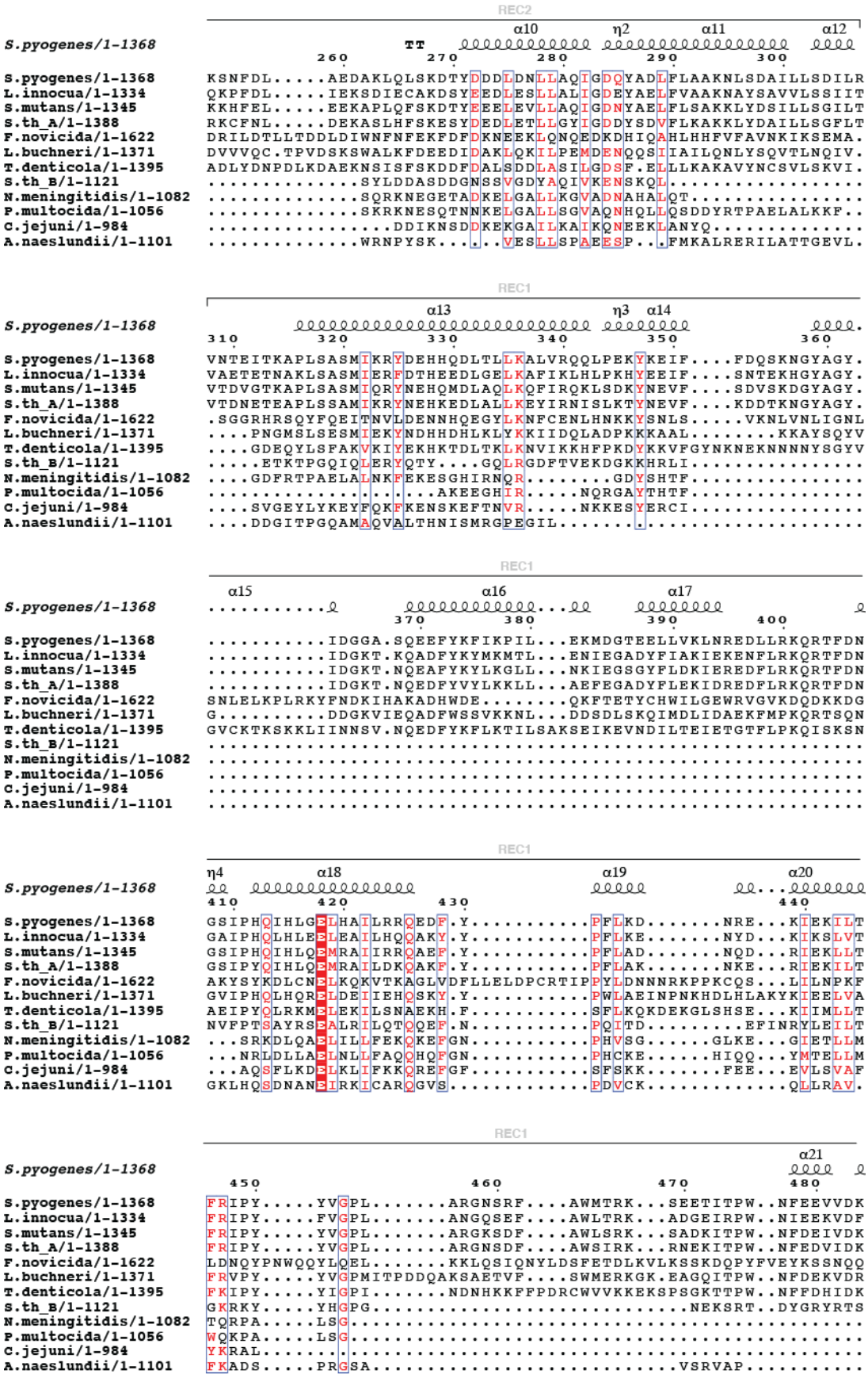
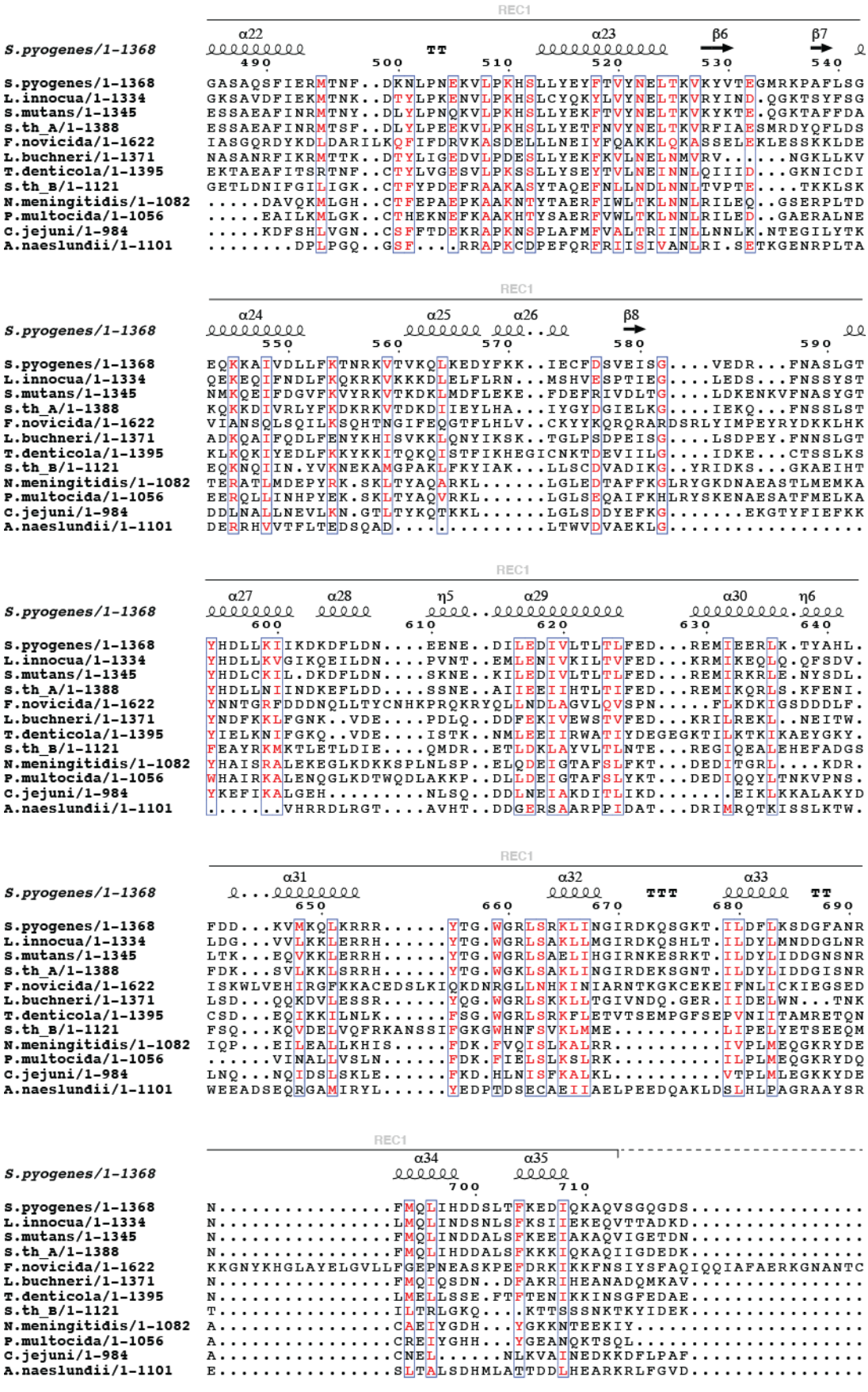
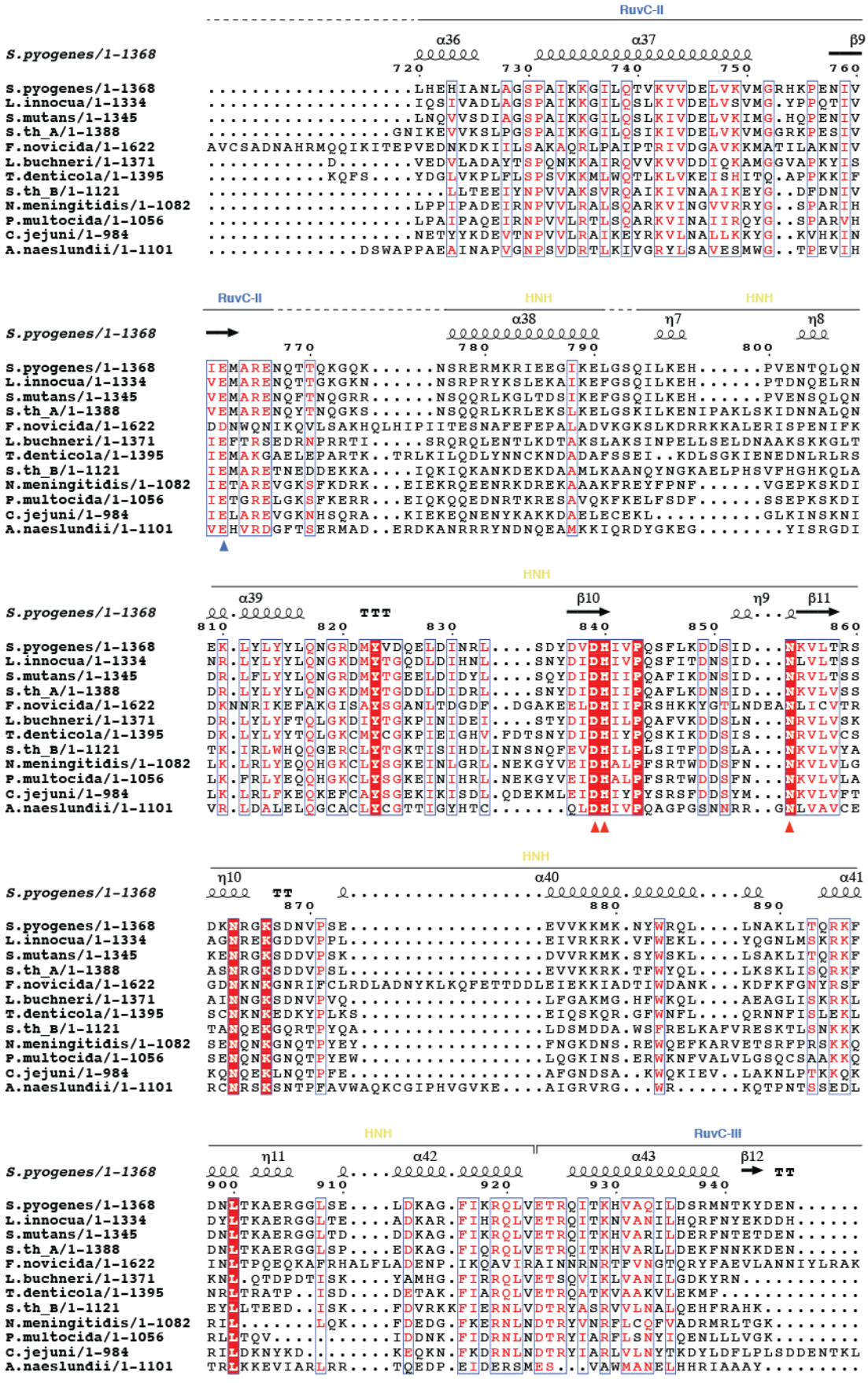
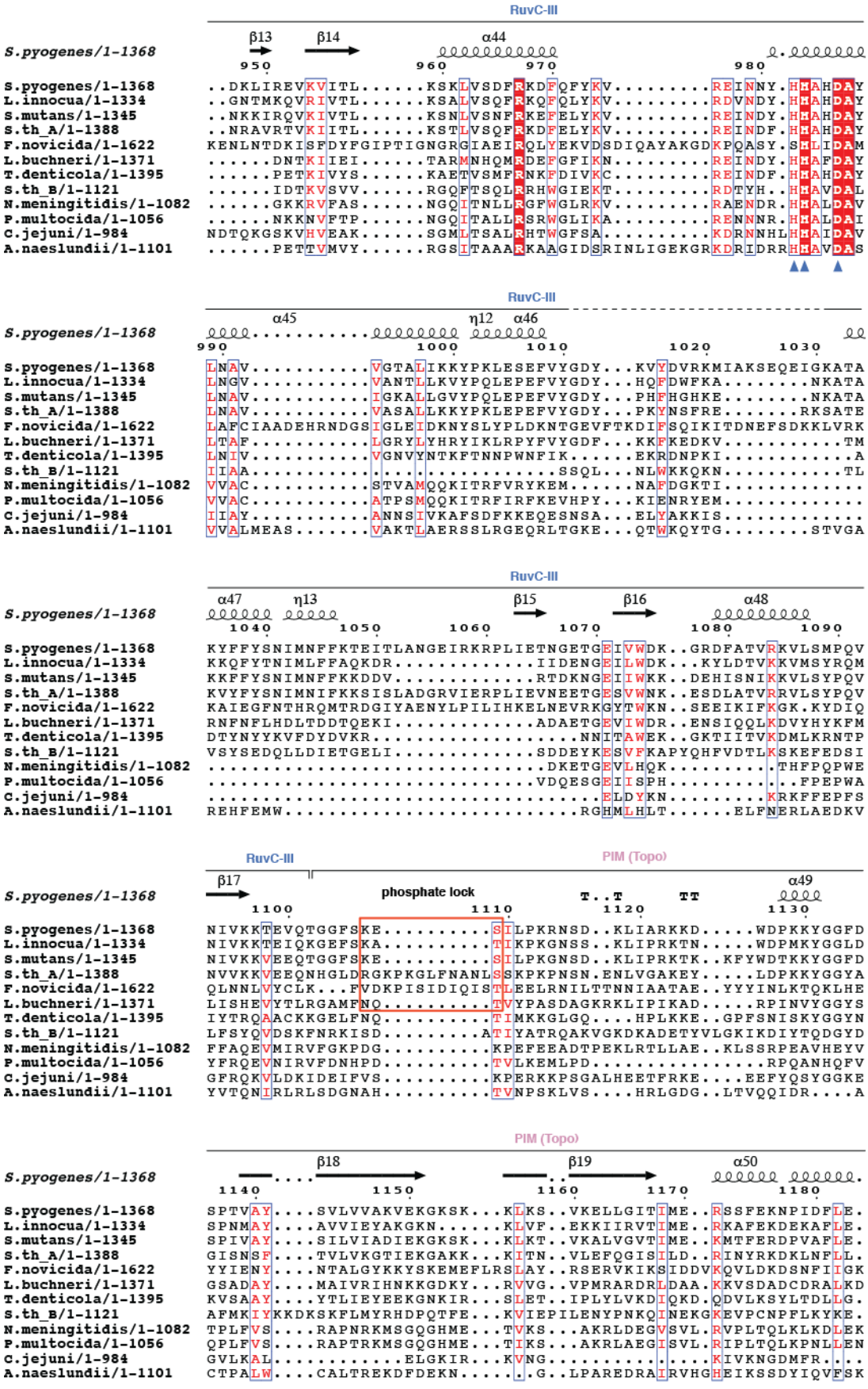
Supplementary Figure 1 | Multiple sequence alignment of Cas9 orthologs. Primary sequences of type II-A Cas9 proteins from *Streptococcus pyogenes* (GI 15675041), *Listeria innocua* Clip 11262 (GI 16801805), *Streptococcus mutans* UA159 (GI 24379809), *Streptococcus thermophilus* LMD-9 (S.thermophilus A, GI 11662823; S.thermophilus B, GI 116627542), *Lactobacillus buchneri* NRRL B-30929 (GI 331702228), *Treponema denticola* ATCC 35405 (GI 42525843), *Francisella novicida* U112 (GI 118497352), *Campylobacter jejuni* subsp. *Jejuni* NCTC 11168 (GI 218563121), *Pasteurella multocida* subsp. *multocida* str. Pm70 (GI 218767588), *Neisseria meningitidis* Zs491 (GI 15602992) and *Actinomyces naeslundii* (GI 489880078) were aligned using MAFFT[36]. The alignment was generated in ESPript (http://espript.ibcp.fr/ESPript/) using default settings. Strictly conserved residues are shown with white letters on red background. Residues with >70% similarity are shown in red and boxed in blue. The domain organization of SpyCas9 and secondary structure are shown above the sequences. Disordered segments of the polypeptide chain are indicated with dashed lines. RuvC domain catalytic residues are denoted with blue arrowheads. HNH domain active site residues are denoted with red arrowheads. PAM-interacting residues contacting the major groove are denoted with black arrowheads. The phosphate lock loop is marked with a red box. PIM; PAM interacting domain.

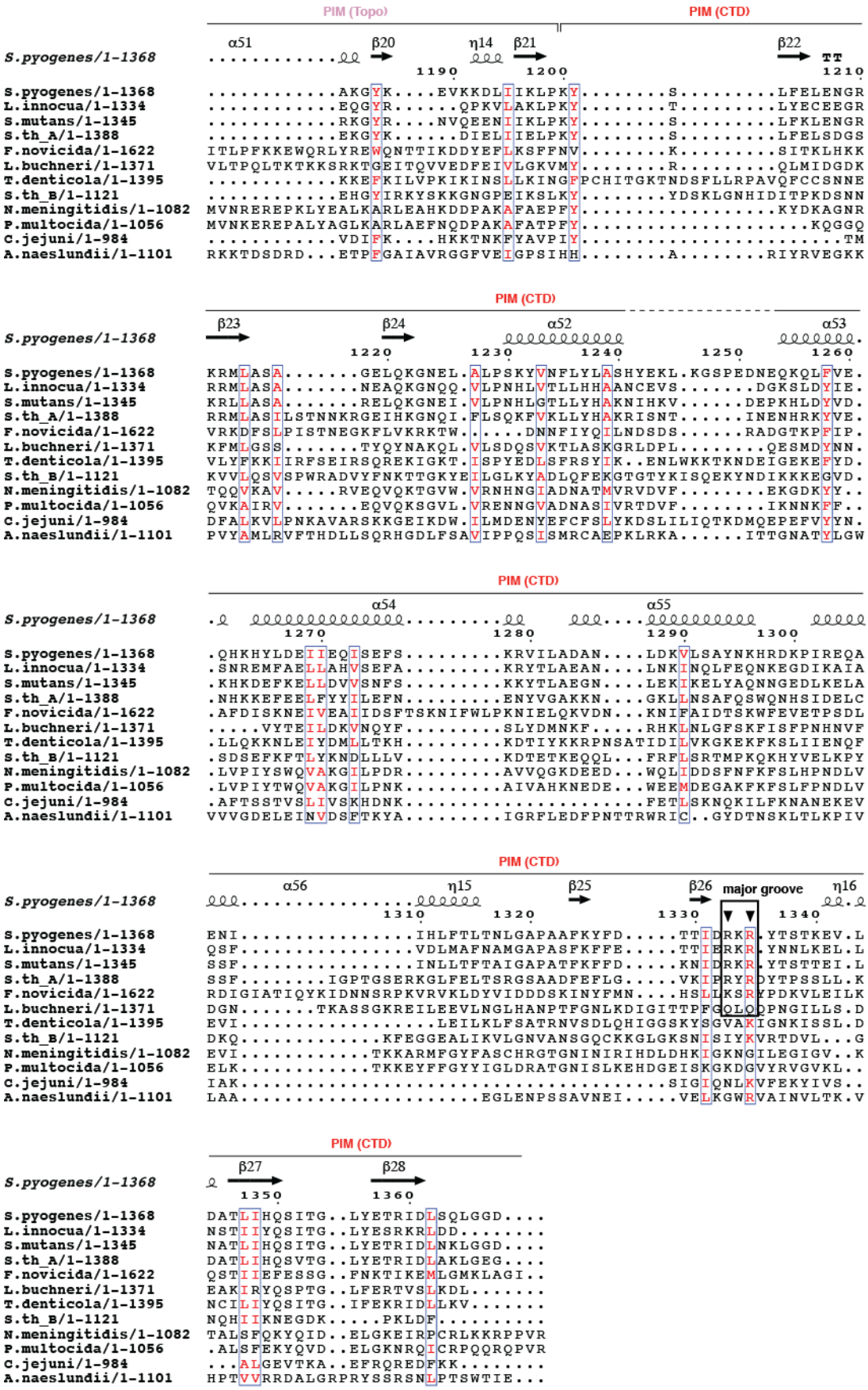

RuvC-I
β1 β2 β3 β4 β5
S.pyogenes/1-1368
1 10 20 30 40 50
S.pyogenes/1-1368 ....MDKK...YSIGLDIGTNSVG.WAVITDEYKVPSKKFKVLGNTDRHSIKKNLIGALL
L.innocua/1-1334 ....MKKP...YTIGLDIGTNSVG.WAVLTDQYDLVKRKMKIAGDSEKKQIKKNFWGVRL
S.mutans/1-1345 ....MKKP...YSIGLDIGTNSVG.WAVVTDDYKVPAKKMKVLGNTDKSHIEKNLLGALL
S.th_A/1-1388 ....MTKP...YSIGLDIGTNSVG.WAVTTDNYKVPSKKMKVLGNTSKKYIKKNLLGVLL
F.novicida/1-1622 ....MNFKI..LPIAIDLGVKNTGVFSAFYQKGTSLE..............RLDNKNGKV
L.buchneri/1-1371 ....MKVNN..YHIGLDIGTSSIG.WVAIGEDGKPLRIK.............GKTAIGARL
T.denticola/1-1395 ....MKKEIKDYFLGLDVGTGSVG.WAVTDTDYKLLKAN.............RKDLWGMRC
S.th_B/1-1121 ....MSD....LVLGLDIGIGSVG.VGILNKVTGE..................IIHKNSRI
N.meningitidis/1-1082 .MAAFKPNPINYILGLDIGIASVG.WAMVEIDEDENPI.............CLIDLGVRV
P.multocida/1-1056 ....MQTTNLSYILGLDLGIASVG.WAVVEINENEDPI.............GLIDVGVRI
C.jejuni/1-984 ....MAR.....ILAFDIGISSIG.WAFSEND...................ELKDCGVRI
A.naeslundii/1-1101 MWYASLMSAHHLRVGIDVGTHSVG.LATLRVDDHGTPI.............ELLSALSHI
Arg-rich
REC1
α1
S.pyogenes/1-1368
60 70 80 90
S.pyogenes/1-1368 FDSGETAEA.......TRL...KRTARRRYTRRKNRICYLQEIFSNEMAKV.DD......
L.innocua/1-1334 FDEGQTAAD.......RRM...ARTARRRIERRRNRISYLQGIFAEEMSKT.DA......
S.mutans/1-1345 FDSGNTAED.......RRL...KRTARRRYTRRRNRILYLQEIFSEEMGKV.DD......
S.th_A/1-1388 FDSGITAEG.......RRL...KRTARRRYTRRRNRILYLQEIFSTEMATL.DD......
F.novicida/1-1622 YELSKDSYT..LLMNNRTA...RRHQRRGIDRKQLVKRLFKLIWTEQLNLEWDKDTQQAI
L.buchneri/1-1371 FQEGNPAAD.......RRM...FRTTRRRLSRRKWRLKLLEEIFDPYITPV.DS......
T.denticola/1-1395 FETAETAEV.......RRL...HRGARRRIERRKKRIKLLQELFSQEIAKT.DE......
S.th_B/1-1121 FPAAQAENN.....LVRRT...NRQGRRLARRKKHRRVRLNRLFEES.GLI.T.......
N.meningitidis/1-1082 FERAEVPKTGDSLAMARRL...ARSVRRLTRRAHRLLRARRLLKREGVLQ.AA......
P.multocida/1-1056 FERAEVPKTGESLALSRRL...ARSTRRLIRRAHRLLLAKRFLKRE.............
C.jejuni/1-984 FTKVENPKTGESLALPRRL...ARSARKRLARRKARLNHLKHLIANE.FKL.NY......
A.naeslundii/1-1101 HDSGVGKEGKKDHDTRKKLSGIARRARRLLHHRRTQLQQLDEVLRDLGFPIPTP......
REC1
α2 α3 α4
S.pyogenes/1-1368
100 110 120 130 140 150
S.pyogenes/1-1368 SFFHRLEES.FLVEEDKKHERHPIFGNIV.DEVAYHEKYP.TIYHLRKKLVDSTDKADLR
L.innocua/1-1334 NFFCRLSDS.FYVDNEKRNSRHPFFATIE.EEVEYHKNYP.TIYHLREELVNSSEKADLR
S.mutans/1-1345 SFFHRLEDS.FLVTEDKRGERHPIFGNLE.EEVKYHENFP.TIYHLRQYLADNPEKVDLR
S.th_A/1-1388 AFFQRLDDS.FLVPDDKRDSKYPIFGNLV.EEKAYHDEFP.TIYHLRKYLADSTKKADLR
F.novicida/1-1622 SFLFNRRGFSFITDGYSPEYLNIVPEQVKAILMDIFDDYN.GEDDLDSYLKLATEQESKI
L.buchneri/1-1371 TFFARLKQSNLSPKDSRKEFKGSMLFPDL.TDMQYHKDYP.TIYHLRHALMTQDEKFDIR
T.denticola/1-1395 GFFQRMKESPFYAEDKTILQENTLFNDKDFADKTYHKAYP.TINHLIKAWIENKVKPDPR
S.th_B/1-1121 .DFTK.....ISINL.NPYQLRVKGLT..DELSNE
N.meningitidis/1-1082 DF.....DENGLIKSLPNTPWQLRAAALD..RKLTPL
P.multocida/1-1056 GIL.....STIDLEKGLPNQAWELRVAGLE..RRLSAI
C.jejuni/1-984 EDYQSFDES.....LAKAYKGSLI.SPYELRFRALN..ELLSKQ
A.naeslundii/1-1101 GEFLDLNEQ.....TDPYRVWRVRARLVEEKLPEELR
REC1
REC2
α5 η1 α6
S.pyogenes/1-1368
160 170 180 190 200
S.pyogenes/1-1368 ..LIYLALAHMIKFRGHFLIE...GDLNPDNSDVDKLFIQLVQTYNQLFEENP......I
L.innocua/1-1334 ..LVYLALAHIIKYRGNFLIE...GALDTQNTSVDGIYKQFIQTYNQVFASGIEDGSLKK
S.mutans/1-1345 ..LVYLALAHIIKFRGHFLIE...GKFDTRNNDVQRLFQEFLAVYDNTFENSS......L
S.th_A/1-1388 ..LVYLALAHMIKYRGHFLIE...GEFNSKNNDIQKNFQDFLDTYNAIFESDL......S
F.novicida/1-1622 SEIYNKLMQKILEFKLMKLCT......DIKDDKVSTKTLKEITSYEFEL..........L
L.buchneri/1-1371 ..MVYLAIHHIVKYRGNFLNSTPVDSFKASKVNFVDQFKKLNELYTAINPEESFQI...N
T.denticola/1-1395 ..LLYLACHNIIKKRGHFLFE...GDFDSEN.....QFDTSIQALFEYLREDMEVDI
S.th_B/1-1121 ..ELFIALKNMVKHRGI.....
N.meningitidis/1-1082 ..EWSAVLLHLIKHRGYL.....
P.multocida/1-1056 ..EWGAVLLHLIKHRGYL.....
C.jejuni/1-984 ..DFARVILHIAKRRGY.....
A.naeslundii/1-1101 GPAISMAVRHIARHRG.....
REC2
α7 α8 α9
S.pyogenes/1-1368
210 220 230 240 250
S.pyogenes/1-1368 NASGVDAKAILSA....RLSKSRRLENLIAQLPGEK.....KNGLFGNLIALSLGLTPNF
L.innocua/1-1334 LEDNKDVAKILVE....KVTRKEKLERILKLYPGEK.....SAGMFAQFISLIVGSKGNF
S.mutans/1-1345 QEQNVQVEEILTD....KISKSAKKDRVLKLFPNEK.....SNGRFAEFLKLIVGNQADF
S.th_A/1-1388 LENSKQLEEIVKD....KISKLEKKDRILKLFPGEK.....NSGIFSEFLKLIVGNQADF
F.novicida/1-1622 ADYLANYSESLKTQKFSYTDKQGNLKELSYYHHDKY.....NIQEFLKRHATIN
L.buchneri/1-1371 LANSEDIGHQFLDPSIRKFDKKKQIPKIVPVSVDDKATDKINGKIASEIINAILGYKSKL
T.denticola/1-1395 DADSQKVKEILKDSSLKNSEKQSRLNKILGLKPSDK.....QKKAITNLIS...GNKINF
S.th_B/1-1121 .....
N.meningitidis/1-1082 .....
P.multocida/1-1056 .....
C.jejuni/1-984 .....
A.naeslundii/1-1101 .....


REC2
α10
η2
α11
α12
S.pyogenes/1-1368
260
270
280
290
300
S.pyogenes/1-1368 KSNFDL.....AEDAKLQLSKDTYDDDLDNLLAQIGDQYADLFLAAKNLSDAILLSDILR
L.innocua/1-1334 QKPFDL.....IEKSDIECAKDSYEEDLESLLALIGDEYAELFVAAKNAYSAVVLSSIIT
S.mutans/1-1345 KKHFEL.....EEKAPLQFSKDTYEEELEVLLAQIGDNYAELFLSAKKLYDSILLSGILT
S.th_A/1-1388 RKCFNL.....DEKASLHFSKESYDEDLETLLGYIGDDYSDVFLKAKKLYDAILLSGFLT
F.novicida/1-1622 DRILDTLLTDDLDIWNFNFEKFDFDKNEEKLQNQEDKDHIQAHLHHFVFAVNKIKSEMA.
L.buchneri/1-1371 DVVVQC.TPVDSKSWALKFDEEDIDAKLQKILPEMDENQQSIIAILQNLYSQVTLNQIV.
T.denticola/1-1395 ADLYDNPDLKDAEKNSISFSKDDFDALSDDLASILGDSF.ELLLKAKAVYNCSVLSKVI.
S.th_B/1-1121 .............SYLDDASDDGNSSVGDYAQIVKENSKQL...................
N.meningitidis/1-1082 .............SQRKNEGETADKELGALLKGVADNAHALQT.................
P.multocida/1-1056 .............SKRKNESQTNNKELGALLSGVAQNHQLLQSDDYRTPAELALKKF..
C.jejuni/1-984 ..............DDIKNSDDKEKGAILKAIKQNEEKLANYQ.....................
A.naeslundii/1-1101 .............WRNPYSK....V.ESLLSPAEESP..FMKALRERILATTGEVL.
REC1
α13
η3
α14
S.pyogenes/1-1368
310
320
330
340
350
360
S.pyogenes/1-1368 VNTEITKAPLSASMIKRYDEHHQDLTLLKALVRQQLPEKYKEIF....FDQSKNGYAGY.
L.innocua/1-1334 VAETETNAKLSASMIERFDTHEEDLGELKAFIKLHLPKHYEEIF....SNTEKHGYAGY.
S.mutans/1-1345 VTDVGTKAPLSASMIQRYNEHQMDLAQLKQFIRQKLSDKYNEVF....SDVSKDGYAGY.
S.th_A/1-1388 VTDNETEAPLSSAMIKRYNEHKEDLALLKEYIRNISLKTYNEVF....KDDTKNGYAGY.
F.novicida/1-1622 .SGGRHRSQYFQEITNVLDENNHQEGYLKNFCENLHNKKYSNLS.....VKNLVNLIGNL
L.buchneri/1-1371 ....PNGMSLSESMIEKYNDHHDHLKLYKKIIDQLADPKKKAAL.........KKAYSQYV
T.denticola/1-1395 ....GDEQYLSFAKVKIYEKHKTDLTKLKNVIKKHFPKDYKKVFGYNKNEKNNNNYSGYV
S.th_B/1-1121 .....ETKTPGQIQLERYQTY....GQLRGDFTVEKDGKKHRLI.................
N.meningitidis/1-1082 ....GDFRTPAELALNKFEKESGHIRNQR.........GDYSHTF.................
P.multocida/1-1056 ..................AKEEGHIR.....NQRGAYTHTF.................
C.jejuni/1-984 ....SVGEYLYKEYFQKFKENSKEFTNVR.....NKKESYERCI.................
A.naeslundii/1-1101 ....DDGITPGQAMAQVALTHNISMRGPEGIL.......................
REC1
α15
α16
α17
S.pyogenes/1-1368
370
380
390
400
S.pyogenes/1-1368 ...........IDGGA.SQEEFYKFIKPIL...EKMDGTEELLVKLNREDLLRKQRTFDN
L.innocua/1-1334 ...........IDGKT.KQADFYKYMKMTL...ENIEGADYFIAKIEKENFLRKQRTFDN
S.mutans/1-1345 ...........IDGKT.NQEAFYKYLKGLL...NKIEGSGYFLDKIEREDFLRKQRTFDN
S.th_A/1-1388 ...........IDGKT.NQEDFYVYLKKLL...AEFEGADYFLEKIDREDFLRKQRTFDN
F.novicida/1-1622 SNLELKPLRKYFNDKIHAKADHWDE.........QKFTETYCHWILGEWRVGVKDQDKKDG
L.buchneri/1-1371 G..........DDGKVIEQADFWSSVKKNL...DDSDLSKQIMDLIDAEKFMPKQRTSQN
T.denticola/1-1395 GVCKTKSKKLIINNSV.NQEDFYKFLKTILSAKSEIKEVNDILTEIETGTFLPKQISKSN
S.th_B/1-1121 ....
N.meningitidis/1-1082 ....
P.multocida/1-1056 ....
C.jejuni/1-984 ....
A.naeslundii/1-1101 ....
REC1
η4
α18
α19
α20
S.pyogenes/1-1368
410
420
430
440
S.pyogenes/1-1368 GSIPHQIHLGELHAILRRQEDF.Y..........PFLKD.......NRE...KIEKILT
L.innocua/1-1334 GAIPHQLHLEELEAILHQQAKY.Y..........PFLKE.......NYD...KIKSLVT
S.mutans/1-1345 GSIPHQIHLQEMRAIIRRQAEF.Y..........PFLAD.......NQD...RIEKLLT
S.th_A/1-1388 GSIPYQIHLQEMRAILDKQAKF.Y..........PFLAK.......NKE...RIEKILT
F.novicida/1-1622 AKYSYKDLCNELKQKVTKAGLVDFLLELDPCRTIPPYLDNNNRKPPKCQS...LILNPKF
L.buchneri/1-1371 GVIPHQLHQRELDEIIEHQSKY.Y..........PWLAEINPNKHDLHLAKYKIEELVA
T.denticola/1-1395 AEIPYQLRKMELEKILSNAEKH.F..........SFLKQKDEKGLSHSE...KIIMLLT
S.th_B/1-1121 NVFPTSAYRSEALRILQTQQEF.N..........PQITD.........EFINRYLEILT
N.meningitidis/1-1082 ...SRKDLQAELILLFEKQKEFGN..........PHVSG......GLKE...GIETLLM
P.multocida/1-1056 ...NRLDLLAELNLLFAQQHQFGN..........PHCKE......HIQQ...YMTELLM
C.jejuni/1-984 ...AQSFLKDELKLIFKKQREFGF..........SFSKK.......FEE...EVLSVAF
A.naeslundii/1-1101 GKLHQSDNANEIRKICARQGVS..........PDVCK.............QLLRAV.
REC1
α21
S.pyogenes/1-1368
450
460
470
480
S.pyogenes/1-1368 FRIPY.....YVGPL.......ARGNSRF....AWMTRK...SEETITPW..NFEEVVDK
L.innocua/1-1334 FRIPY.....FVGPL.......ANGQSEF....AWLTRK...ADGEIRPW..NIEEKVDF
S.mutans/1-1345 FRIPY.....YVGPL.......ARGKSDF....AWLSRK...SADKITPW..NFDEIVDK
S.th_A/1-1388 FRIPY.....YVGPL.......ARGNSDF....AWSIRK...RNEKITPW..NFEDVIDK
F.novicida/1-1622 LDNQYPNWQQYLQEL.......KKLQSIQNYLDSFETDLKVLKSSKDQPYFVEYKSSNQQ
L.buchneri/1-1371 FRVPY.....YVGPMITPDDQAKSAETVF....SWMERKGK.EAGQITPW..NFDEKVDR
T.denticola/1-1395 FKIPY.....YIGPI.......NDNHKKFFPDRCWVVKKEKSPSGKTTPW..NFFDHIDK
S.th_B/1-1121 GKRKY.....YHGPG.............................NEKSRT..DYGRYRTS
N.meningitidis/1-1082 TQRPA.....LSG..
P.multocida/1-1056 WQKPA.....LSG..
C.jejuni/1-984 YKRAL...
A.naeslundii/1-1101 FKADS.....PRGSA.....................VSRVAP.....


REC1
α22 α23 β6 β7
S.pyogenes/1-1368
490 500 510 520 530 540
S.pyogenes/1-1368 GASAQSFIERMTNF..DKNLPNEKVLPKHSLLYEYFTVYNELTKVKYVTEGMRKPAFLSG
L.innocua/1-1334 GKSAVDFIEKMTNK..DTYLPKENVLPKHSLCYQKYLVYNELTKVRYIND.QGKTSYFSG
S.mutans/1-1345 ESSAEAFINRMTNY..DLYLPNQKVLPKHSLLYEKFTVYNELTKVKYKTE.QGKTAFFDA
S.th_A/1-1388 ESSAEAFINRMTSF..DLYLPEEKVLPKHSLLYETFNVYNELTKVRFIAESMRDYQFLDS
F.novicida/1-1622 IASGQRDYKDLDARILKQFIFDRVKASDELLLNEIYFQAKKLQKASSELEKLESSKKLDE
L.buchneri/1-1371 NASANRFIKRMTTK..DTYLIGEDVLPDESLLYEKFKVLNELNMVRV.....NGKLLKV
T.denticola/1-1395 EKTAEAFITSRTNF..CTYLVGESVLPKSSLLYSEYTVLNEINNLQIIID...GKNICDI
S.th_B/1-1121 GETLDNIFGILIGK..CTFYPDEFRAAKASYTAQEFNLLNDLNNLTVPTE....TKKLSK
N.meningitidis/1-1082 .....DAVQKMLGH..CTFEPAEPKAAKNTYTAERFIWLTKLNNLRILEQ..GSERPLTD
P.multocida/1-1056 .....EAILKMLGK..CTHEKNEFKAAKHTYSAERFVWLTKLNNLRILED..GAERALNE
C.jejuni/1-984 .....KDFSHLVGN..CSFFTDEKRAPKNSPLAFMFVALTRIINLLNNLK.NTEGILYTK
A.naeslundii/1-1101 .....DPLPGQ..GSF...RRAPKCDPEFQRFRIISIVANLRI.SETKGENRPLTA
REC1
α24 α25 α26 β8
S.pyogenes/1-1368
550 560 570 580 590
S.pyogenes/1-1368 EQKKAIVDLLFKTNRKVTVKQLKEDYFKK..IECFDSVEISG....VEDR...FNASLGT
L.innocua/1-1334 QEKEQIFNDLFKQKRKVKKKDLELFLRN...MSHVESPTIEG....LEDS...FNSSYST
S.mutans/1-1345 NMKQEIFDGVFKVYRKVTKDKLMDFLEKE..FDEFRIVDLTG....LDKENKVFNASYGT
S.th_A/1-1388 KQKKDIVRLYFKDKRKVTDKDIIEYLHA...IYGYDGIELKG....IEKQ...FNSSLST
F.novicida/1-1622 VIANSQLSQILKSQHTNGIFEQGTFLHLV..CKYYKQRQRARDSRLYIMPEYRYDKKLHK
L.buchneri/1-1371 ADKQAIFQDLFENYKHISVKKLQNYIKSK..TGLPSDPEISG....LSDPEY.FNNSLGT
T.denticola/1-1395 KLKQKIYEDLFKKYKKITQKQISTFIKHEGICNKTDEVIILG....IDKE...CTSSLKS
S.th_B/1-1121 EQKNQIIN.YVKNEKAMGPAKLFKYIAK...LLSCDVADIKG..YRIDKS...GKAEIHT
N.meningitidis/1-1082 TERATLMDEPYRK.SKLTYAQARKL.....LGLEDTAFFKGLRYGKDNAEASTLMEMKA
P.multocida/1-1056 EERQLLINHPYEK.SKLTYAQVRKL.....LGLSEQAIFKHLRYSKENAESATFMELKA
C.jejuni/1-984 DDLNALLNEVLKN.GTLTYKQTKKL.....LGLSDDYEFKG.....EKGTYFIEFKK
A.naeslundii/1-1101 DERRHVVTFLTEDSQAD....LTWVDVAEKLG.....
REC1
α27 α28 η5 α29 α30 η6
S.pyogenes/1-1368
600 610 620 630 640
S.pyogenes/1-1368 YHDLLKIIKDKDFLDN....EENE..DILEDIVLTLTLFED...REMIEERLK.TYAHL.
L.innocua/1-1334 YHDLLKVGIKQEILDN....PVNT..EMLENIVKILTVFED...KRMIKEQLQ.QFSDV.
S.mutans/1-1345 YHDLCKILDKDFLDN....SKNE..KILEDIVLTLTLFED...REMIRKRLE.NYSDL.
S.th_A/1-1388 YHDLLNIINDKEFLDD....SSNE..AIIEEIIHTLTIFED...REMIKQRLS.KFENI.
F.novicida/1-1622 YNNTGRFDDDNQLLTYCNHKPRQKRYQLLNDLAGVLQVSPN.....FLKDKIGSDDDLF.
L.buchneri/1-1371 YNDFKKLFGNK..VDE....PDLQ..DDFEKIVEWSTVFED...KRILREKL..NEITW.
T.denticola/1-1395 YIELKNIFGKQ..VDE....ISTK..NMLEEIIRWATIYDEGEGKTILKTKIKAEYGKY.
S.th_B/1-1121 FEAYRKMKTLETLDIE....QMDR..ETLDKLAYVLTLNTE...REGIQEALEHEFADGS
N.meningitidis/1-1082 YHAISRALEKEGLKDKKSPLNLSP..ELQDEIGTAFSLFKT...DEDITGRL....KDR.
P.multocida/1-1056 WHAIRKALENQGLKDTWQDLAKKP..DLLDEIGTAFSLYKT...DEDIQQYLTNKVPNS.
C.jejuni/1-984 YKEFIKALGEH.....NLSQ..DDLNEIAKDITLIKD.....EIKLKKALAKYD
A.naeslundii/1-1101 .....VHRRDLRGT....AVHT..DDGERSAARPPIDAT...DRIMRQTKISSLKTW.
REC1
α31 α32 α33
S.pyogenes/1-1368
650 660 670 680 690
S.pyogenes/1-1368 FDD...KVMKQLKRRR.....YTG.WGRLSRKLINGIRDKQSGKT.ILDFLKSDGFANR
L.innocua/1-1334 LDG...VVLKKLERRH.....YTG.WGRLSAKLLMGIRDKQSHLT.ILDYLMNDDGLNR
S.mutans/1-1345 LTK...EQVKKLERRH.....YTG.WGRLSAELIHGIRNKESRKT.ILDYLIDDGNSNR
S.th_A/1-1388 FDK...SVLKKLSRRH.....YTG.WGKLSAKLINGIRDEKSGNT.ILDYLIDDGISNR
F.novicida/1-1622 ISKWLVEHIRGFKKACEDSLKIQKDNRGLLNHKINIARNTKGKCEKEIFNLICKIEGSED
L.buchneri/1-1371 LSD...QQKDVLESSR.....YQG.WGRLSKKLLTGIVNDQ.GER.IIDELWN...TNK
T.denticola/1-1395 CSD...EQIKKILNLK.....FSG.WGRLSRKFLETVTSEMPGFSEPVNIITAMRETQN
S.th_B/1-1121 FSQ...KQVDELVQFRKANSSIFGKGWHNFSVKLMME.....LIPELYETSEEQM
N.meningitidis/1-1082 IQP...EILEALLKHIS.....FDK.FVQISLKALRR.....IVPLMEQGKRYDE
P.multocida/1-1056 .....VINALLVSLN.....FDK.FIELSLKSLRK.....ILPLMEQGKRYDQ
C.jejuni/1-984 LNQ...NQIDSLSKLE.....FKD.HLNISFKALKL.....VTPLMLEGKKYDE
A.naeslundii/1-1101 WEEADSEQRGAMIRYL.....YEDPTDSECAEIIAELPEEDQAKLDSLHLPAGRAAYSR
REC1
α34 α35
S.pyogenes/1-1368
700 710
S.pyogenes/1-1368 N.....FMQLIHDDSLTFKEDIQKAQVSGQGDS.....
L.innocua/1-1334 N.....LMQLINDSNLSFKSIIEKEQVTTADKD.....
S.mutans/1-1345 N.....FMQLINDDALSFKEEIAKAQVIGETDN.....
S.th_A/1-1388 N.....FMQLIHDDALSFKKKIQKAQIIGDEDK.....
F.novicida/1-1622 KKGNYKHGLAYELGVLLFGEPNEASKPEFDRKIKKFNSIYSFAQIQQIAFAERKGNANTC
L.buchneri/1-1371 N.....FMQIQSDN..DFAKRIHEANADQMKAV.....
T.denticola/1-1395 N.....LMELLSSE.FTFTENIKKINSGFEDAE.....
S.th_B/1-1121 T.....ILTRLGKQ....KTTSSSNKTKYIDEK.....
N.meningitidis/1-1082 A.....CAEIYGDH...YGKKNTEEKIY.....
P.multocida/1-1056 A.....CREIYGHH...YGEANQKTSQL.....
C.jejuni/1-984 A.....CNEL.....NLKVAINEDKKDFLPAF.....
A.naeslundii/1-1101 E.....SLTALSDHMLATTDDLHEARKRLFGVD.....


RuvC-II
α36
α37
β9
S.pyogenes/1-1368
720
730
740
750
760
S.pyogenes/1-1368 ..................LHEHIANLAGSPAIKKGILQTVKVVDELVKVMGRHKPENIV
L.innocua/1-1334 ..................IQSIVADLAGSPAIKKGILQSLKIVDELVSVMG.YPPQTIV
S.mutans/1-1345 ..................LNQVVSDIAGSPAIKKGILQSLKIVDELVKIMG.HQPENIV
S.th_A/1-1388 ..................GNIKEVVKSLPGSPAIKKGILQSIKIVDELVKVMGGRKPESIV
F.novicida/1-1622 AVCSADNAHRMQQIKITEPVEDNKDKIILSAKAQRLPAIPTRIVDGAVKKMATILAKNIV
L.buchneri/1-1371 ....D.......VEDVLADAYTSPQNKKAIRQVVKVVDDIQKAMGGVAPKYIS
T.denticola/1-1395 ..........KQFS....YDGLVKPLFLSPSVKKMLWQTLKLVKEISHITQ.APPKKIF
S.th_B/1-1121 .....................LLTEEIYNPVVAKSVRQAIKIVNAAIKEYG..DFDNIV
N.meningitidis/1-1082 ..................LPPIPADEIRNPVVLRALSQARKVINGVVRRYG..SPARIH
P.multocida/1-1056 ..................LPAIPAQEIRNPVVLRTLSQARKVINAIIRQYG..SPARVH
C.jejuni/1-984 ..................NETYYKDEVTNPVVLRAIKEYRKVLNALLKKYG..KVHKIN
A.naeslundii/1-1101 ..............DSWAPPAEAINAPVGNPSVDRTLKIVGRYLSAVESMWG..TPEVIH
RuvC-II
HNH
HNH
α38
η7
η8
S.pyogenes/1-1368
770
780
790
800
S.pyogenes/1-1368 IEMARENQTTQKGQK......NSRERMKRIEEGIKELGSQILKEH......PVENTQLQN
L.innocua/1-1334 VEMARENQTTGKGKN......NSRPRYKSLEKAIKEFGSQILKEH......PTDNQELRN
S.mutans/1-1345 VEMARENQFTNQGRR......NSQQRLKGLTDSIKEFGSQILKEH......PVENSQLQN
S.th_A/1-1388 VEMARENQYTNQGKS......NSQQRLKRLEKSLKELGSKILKENIPAKLSKIDNNALQN
F.novicida/1-1622 DDNWQNIKQVLSAKHQLHIPIITESNAFEFEPALADVKGKSLKDRRKKALERISPENIFK
L.buchneri/1-1371 IEFTRSEDRNPRRTI.....SRQRQLENTLKDTAKSLAKSINPELLSELDNAAKSKKGLT
T.denticola/1-1395 IEMAKGAELEPARTK..TRLKILQDLYNNCKNDADAFSSEI..KDLSGKIENEDNLRLRS
S.th_B/1-1121 IEMARETNEDDEKKA....IQKIQKANKDEKDAAMLKAANQYNGKAELPHSVFHGHKQLA
N.meningitidis/1-1082 IETAREVGKSFKDRK...EIEKRQEENRKDREKAAAKFREYFPNF......VGEPKSKDI
P.multocida/1-1056 IETGRELGKSFKERR...EIQKQQEDNRTKRESAVQKFKELFSDF......SSEPKSKDI
C.jejuni/1-984 IELAREVGKNHSQRA...KIEKEQNENYKAKKDAELECEKL.........GLKINSKNI
A.naeslundii/1-1101 VEHVRDGFTSERMAD..ERDKANRRRYNDNQEAMKKIQRDYGKEG........YISRGDI
HNH
α39
β10
η9
β11
S.pyogenes/1-1368
TTT
810
820
830
840
850
860
S.pyogenes/1-1368 EK.LYLYYLQNGRDMYVDQELDINRL....SDYDVDHIVPQSFLKDDSID...NKVLTRS
L.innocua/1-1334 NR.LYLYYLQNGKDMYTGQDLDIHNL....SNYDIDHIVPQSFITDNSID...NLVLTSS
S.mutans/1-1345 DR.LFLYYLQNGRDMYTGEELDIDYL....SQYDIDHIIPQAFIKDNSID...NRVLTSS
S.th_A/1-1388 DR.LYLYYLQNGKDMYTGDDLDIDRL....SNYDIDHIIPQAFLKDNSID...NKVLVSS
F.novicida/1-1622 DKNNRIKEFAKGISAYSGANLTDGDF..DGAKEELDHIIPRSHKKYGTLNDEANLICVTR
L.buchneri/1-1371 DR.LYLYFTQLGKDIYTGKPINIDEI....STYDIDHILPQAFVKDDSLN...NRVLVSK
T.denticola/1-1395 DK.LYLYYTQLGKCMYCGKPIEIGHV.FDTSNYDIDHIYPQSKIKDDSIS...NRVLVCS
S.th_B/1-1121 TK.IRLWHQQGERCLYTGKTISIHDLINNSNQFEVDHILPLSITFDDSLA...NKVLVYA
N.meningitidis/1-1082 LK.LRLYEQQHGKCLYSGKEINLGRL.NEKGYVEIDHALPFSRTWDDSFN...NKVLVLG
P.multocida/1-1056 LK.FRLYEQQHGKCLYSGKEINIHRL.NEKGYVEIDHALPFSRTWDDSFN...NKVLVLA
C.jejuni/1-984 LK.LRLFKEQKEFCAYSGEKIKISDL.QDEKMLEIDHIYPYSRSFDDSYM...NKVLVFT
A.naeslundii/1-1101 VR.LDALELQGCACLYCGTTIGYHTC.......QLDHIVPQAGPGSNNRR..GNLVAVCE
HNH
η10
α40
α41
S.pyogenes/1-1368
TT
870
880
890
S.pyogenes/1-1368 DKNRGKSDNVPSE.....................EVVKKMK.NYWRQL....LNAKLITQRKF
L.innocua/1-1334 AGNREKGDDVPPL.....................EIVRKRK.VFWEKL....YQGNLMSKRKF
S.mutans/1-1345 KENRGKSDDVPSK.....................DVVRKMK.SYWSKL....LSAKLITQRKF
S.th_A/1-1388 ASNRGKSDDVPSL.....................EVVKKRK.TFWYQL....LKSKLISQRKF
F.novicida/1-1622 GDNKGNRIFCLRDLADNYKLKQFETTDDLEIEKKIADTIWDANK...KDFKFGNYRSF
L.buchneri/1-1371 AINNGKSDNVPVQ.....................LFGAKMG.HFWKQL....AEAGLISKRKL
T.denticola/1-1395 SCNKNKEDKYPLKS.....................EIQSKQR.GFWNFL....QRNNFISLEKL
S.th_B/1-1121 TANQEKGQRTPYQA.....................LDSMDDA.WSFRELKAFVRESKTLSNKKK
N.meningitidis/1-1082 SENQNKGNQTPYEY.....................FNGKDNS.REWQEFKARVETSRFPRSKKQ
P.multocida/1-1056 SENQNKGNQTPYEW.....................LQGKINS.ERWKNFVALVLGSQCSAAKKQ
C.jejuni/1-984 KQNQEKLNQTPFE.....................AFGNDSA..KWQKIEV..LAKNLPTKKQK
A.naeslundii/1-1101 RCNRSKSNTPFAVWAQKCGIPHVGVKE....AIGRVRG...WR......KQTPNTSSEDL
HNH
RuvC-III
η11
α42
α43
β12
S.pyogenes/1-1368
900
910
920
930
940
S.pyogenes/1-1368 DNLTKAERGGLSE....LDKAG.FIKRQLVETRQITKHVAQILDSRMNTKYDEN......
L.innocua/1-1334 DYLTKAERGGLTE....ADKAR.FIHRQLVETRQITKNVANILHQRFNYEKDDH......
S.mutans/1-1345 DNLTKAERGGLTD....DDKAG.FIKRQLVETRQITKHVARILDERFNTETDEN......
S.th_A/1-1388 DNLTKAERGGLSP....EDKAG.FIQRQLVETRQITKHVARLLDEKFNNKKDEN......
F.novicida/1-1622 INLTPQEQKAFRHALFLADENP.IKQAVIRAINNRNRTFVNGTQRYFAEVLANNIYLRAK
L.buchneri/1-1371 KNL.QTDPDTISK....YAMHG.FIRRQLVETSQVIKLVANILGDKYRN..........
T.denticola/1-1395 NRLTRATP..ISD....DETAK.FIARQLVETRQATKVAAKVLEKMF..........
S.th_B/1-1121 EYLLTEED..ISK....FDVRKKFIERNLVDTRYASRVVLNALQEHFRAHK........
N.meningitidis/1-1082 RILL.......LQK....FDEDG.FKERNLNDTRYVNRFLCQFVADRMRLTGK........
P.multocida/1-1056 RLLTQV.....IDDNK.FIDRNLNDTRYIARFLSNYIQENLLLVGK........
C.jejuni/1-984 RILDKNYKD.....KEQKN.FKDRNLNDTRYIARLVLNYTKDYLDFLPLSDDENTKL
A.naeslundii/1-1101 TRLKKEVIARLRR....TQEDP.EIDERSMES...VAWMANELHHRIAAAY.....


RuvC-III
β13
β14
α44
S.pyogenes/1-1368
950
960
970
980
S.pyogenes/1-1368 ..DKLIREVKVITL.....KSKLVSDFRKDFQFYKV.....REINNY.HHAHDAY
L.innocua/1-1334 ..GNTMKQVRIVTL.....KSALVSQFRKQFQLYKV.....RDVNDY.HHAHDAY
S.mutans/1-1345 ..NKKIRQVKIVTL.....KSNLVSNFRKEFELYKV.....REINDY.HHAHDAY
S.th_A/1-1388 ..NRAVRTVKIITL.....KSTLVSQFRKDFELYKV.....REINDF.HHAHDAY
F.novicida/1-1622 KENLNTDKISFDYFGIPTIGNGRGIAEIRQLYEKVDSDIQAYAKGDKPQASY.SHLIDAM
L.buchneri/1-1371 .....DNTKIIEI.....TARMNHQMRDEFGFIKN.....REINDY.HHAFDAY
T.denticola/1-1395 .....PETKIVYS.....KAETVSMFRNKFDIVKC.....REINDF.HHAHDAY
S.th_B/1-1121 .....IDTKVSVV.....RGQFTSQLRRHWGIEKT.....RDTYH..HHAVDAL
N.meningitidis/1-1082 .....GKKRVFAS.....NGQITNLLRGFWGLRKV.....RAENDR.HHALDAV
P.multocida/1-1056 .....NKKNVFTP.....NGQITALLRSRWGLIKA.....RENNNR.HHALDAI
C.jejuni/1-984 NDTQKGSKVHVEAK.....SGMLTSALRHTWGFSA.....KDRNNHLHHAIDAV
A.naeslundii/1-1101 .....PETTVMVY.....RGSITAAARKAAGIDSRINLIGEKGRKDRIDRRHHAVDAS
RuvC-III
α45
η12
α46
S.pyogenes/1-1368
990
1000
1010
1020
1030
S.pyogenes/1-1368 LNAV.....VGTALIKKYPKLESEFVYGDY...KVYDVRKMIAKSEQEIGKATA
L.innocua/1-1334 LNGV.....VANTLLKVYPQLEPEFVYGDY...HQFDWFKA.....NKATA
S.mutans/1-1345 LNAV.....IGKALLGVYPQLEPEFVYGDY...PHFHGHKE.....NKATA
S.th_A/1-1388 LNAV.....VASALLKKYPKLEPEFVYGDY...PKYNSFRE.....RKSATE
F.novicida/1-1622 LAFCIAADEHRNDGSIGLEIDKNYSLYPLDKNTGEVFTKDIFSQIKITDNEFSDKKLVRK
L.buchneri/1-1371 LTAF.....LGRYLYHRYIKLRPYFVYGDF...KKFKEDKV.....TM
T.denticola/1-1395 LNIV.....VGNVYNTKFTNNPWNFIK.....EKRDNPKI.....A
S.th_B/1-1121 IIAA.....SSQL...NLWKKQKN.....TL
N.meningitidis/1-1082 VVAC.....STVAMQQKITRFVRYKEM.....NAFDGKTI.....
P.multocida/1-1056 VVAC.....ATPSMQQKITRFIRFKEVHPY...KIENRYEM.....
C.jejuni/1-984 IIAY.....ANNSIVKAFSDFKKEQESNSA...ELYAKKIS.....
A.naeslundii/1-1101 VVALMEAS.....VAKTLAERSSLRGEQRLTGKE...QTWKQYTG.....STVGA
RuvC-III
α47
η13
β15
β16
α48
S.pyogenes/1-1368
1040
1050
1060
1070
1080
1090
S.pyogenes/1-1368 KYFFYSNIMNFFKTEITLANGEIRKRPLIETNGETGEIVWDK..GRDFATVRKVLSMPQV
L.innocua/1-1334 KKQFYTNIMLFFAQKDR.....IIDENGEILWDK...KYLDTVKKVMSYRQM
S.mutans/1-1345 KKFFYSNIMNFFKKDDV.....RTDKNGEIIWKK..DEHISNIKKVLSYPQV
S.th_A/1-1388 KVYFYSNIMNIFKKSISLADGRVIERPLIEVNEETGESVWNK..ESDLATVRRVLSYPQV
F.novicida/1-1622 KAIEGFNTHRQMTRDGIYAENYLPILIHKELNEVRKGYTWKN..SEEIKIFKGK.KYDIQ
L.buchneri/1-1371 RNFNFLHDLTDDTQEKI.....ADAETGEVIWDR..ENSIQQLKDVYHYKFM
T.denticola/1-1395 DTYNYYKVFDYDVKR.....NNITAWEK..GKTIITVKDMLKRNTP
S.th_B/1-1121 VSYSEDQLLDIETGELI.....SDDEYKESVFKAPYQHFVDTLKSKEFEDSI
N.meningitidis/1-1082 .....DKETGEVLHQK.....THFPQPWE
P.multocida/1-1056 .....VDQESGEIISPH.....FPEPWA
C.jejuni/1-984 .....ELDYKN.....KRKFFEPFS
A.naeslundii/1-1101 REHFEMW.....RGHMLHLT.....ELFNERLAEDKV
RuvC-III
PIM (Topo)
β17
phosphate lock
T..T
TT
α49
S.pyogenes/1-1368
1100
1110
1120
1130
S.pyogenes/1-1368 NIVKKTEVQTGGFSKE.....SILPKRNSD..KLIARKKD.....WDPKKYGGFD
L.innocua/1-1334 NIVKKTEIQKGEFSKA.....TIKPKGNSS..KLIPRKTN.....WDPMKYGGLD
S.mutans/1-1345 NIVKKVEEQTGGFSKE.....SILPKGNSD..KLIPRKTK..KFYWDTKKYGGFD
S.th_A/1-1388 NVVKKVEEQNHGLDRGKPKGLFNANLSSKPKPNSN.ENLVGAKEY.....LDPKKYGGYA
F.novicida/1-1622 QLNNLVYCLK...FVDKPISIDIQISTLEELRNILTTNNIAATAE..YYYINLKTQKLHE
L.buchneri/1-1371 LISHEVYTLRGAMFNQ.....TVYPASDAGKRKLIPIKAD.....RPINVYGGYS
T.denticola/1-1395 IYTRQAACKKGELFNQ.....TIMKKGLGQ....HPLKKE..GPFSNISKYGGYN
S.th_B/1-1121 LFSYQVDSKFNRKISD.....ATIYATRQAKVGKDKADETYVLGKIKDIYTQDGYD
N.meningitidis/1-1082 FFAQEVMIRVFGKPDG.....KPEFEEADTPEKLRTLLAE..KLSSRPEAVHEYV
P.multocida/1-1056 YFRQEVNIRVFDNHPD.....TVLKEMLPD.....RPQANHQFV
C.jejuni/1-984 GFRQKVLDKIDEIFVS.....KPERKKPSGALHEETFRKE....EEFYQSYGGKE
A.naeslundii/1-1101 YVTQNIRLRLSDGNAH.....TVNPSKLVS....HRLGDG..LTVQQIDR....A
PIM (Topo)
β18
β19
α50
S.pyogenes/1-1368
1140
1150
1160
1170
1180
S.pyogenes/1-1368 SPTVAY....SVLVVAKVEKGKSK...KLKS..VKELLGITIME..RSSFEKNPIDFLE.
L.innocua/1-1334 SPNMAY....AVVIEYAKGKN.....KLVF..EKKIIRVTIME..RKAFEKDEKAFLE.
S.mutans/1-1345 SPIVAY....SILVIADIEKGKSK...KLKT..VKALVGVTIME..KMTFERDPVAFLE.
S.th_A/1-1388 GISNSF....TVLVKGTIEKGAKK...KITN..VLEFQGISILD..RINYRKDKLNFLL.
F.novicida/1-1622 YYIENY....NTALGYKKYSKEMEFLRSLAY..RSERVKIKSIDDVKQVLDKDSNFIIGK
L.buchneri/1-1371 GSADAY....MAIVRIHNKKGDKY...RVVG..VPMRARDRLDAA.KKVSDADCDRALKD
T.denticola/1-1395 KVSAAY....YTLIEYEEKGNKIR...SLET..IPLYLVKDIQKD.QDVLKSYLTDLLG.
S.th_B/1-1121 AFMKIYKKDKSKFLMYRHDPQTFE...KVIEPILENYPNKQINEKGKEVPCNPFLKYKE.
N.meningitidis/1-1082 TPLFVS....RAPNRKMSGQGHME...TVKS...AKRLDEGVSVL.RVPLTQLKLKDLEK
P.multocida/1-1056 QPLFVS....RAPTRKMSGQGHME...TIKS...AKRLAEGISVL.RIPLTQLKPNLLEN
C.jejuni/1-984 GVLKAL.....ELGKIR...KVNG.....KIVKNGDMFR....
A.naeslundii/1-1101 CTPALW....CALTREKDFDEKN.....G..LPAREDRAIRVHGHEIKSSDYIQVFSK


PIM (Topo)
PIM (CTD)
α51
β20
η14
β21
β22
TT
S.pyogenes/1-1368
1190
1200
1210
S.pyogenes/1-1368 .....AKGYK....EVKKDLIIKLPKY.....S.....LFELENGR
L.innocua/1-1334 .....EQGYR.....QPKVLAKLPKY.....T.....LYECEEGR
S.mutans/1-1345 .....RKGYR....NVQEENIIKLPKY.....S.....LFKLENGR
S.th_A/1-1388 .....EKGYK.....DIELIIELPKY.....S.....LFELSDGS
F.novicida/1-1622 ITLPFKKEWQRLYREWQNTTIKDDYEFLKSFFNV.....K.....SITKLHKK
L.buchneri/1-1371 VLTPQLTKTKKSRKTGEITQVVEDFEIVLGKVMY.....R.....QLMIDGDK
T.denticola/1-1395 .....KKEFKILVPKIKINSLLKINGFPCHITGKTNDSFLLRPAVQFCCSNNE
S.th_B/1-1121 .....EHGYIRKYSKKGNGPEIKSLKY.....YDSKLGNHIDITPKDSNN
N.meningitidis/1-1082 MVNREREPKLYEALKARLEAHKDDPAKAFAEPFY.....KYDKAGNR
P.multocida/1-1056 MVNKEREPALYAGLKARLAEFNQDPAKAFATPFY.....KQGGQ
C.jejuni/1-984 .....VDIFK....HKKTNKFYAVPIY.....TM
A.naeslundii/1-1101 RKKTDSDRD...ETPFGAIAVRGGFVEIGPSIHH.....A.....RIYRVEGKK
PIM (CTD)
β23
β24
α52
α53
1220
1230
1240
1250
1260
S.pyogenes/1-1368 KRMLASA.....GELQKGNEL.ALPSKYVNFLYLASHYEKL.KGSPEDNEQKQLFVE.
L.innocua/1-1334 RRMLASA.....NEAQKGNQQ.VLPNHLVTLLHHAANCEVS.....DGKSLDYIE.
S.mutans/1-1345 KRLLASA.....RELQKGNEI.VLPNHLGTLLYHAKNIHKV.....DEPKHLDYVD.
S.th_A/1-1388 RRMLASILSTNNKRGEIHKGNQI.FLSQKFVKLLYHAKRISNT.....INENHRKYVE.
F.novicida/1-1622 VRKDFSLPISTNEGKFLVKRKTW.....DNNFIYQILNDSDS.....RADGTKPFIP.
L.buchneri/1-1371 KFMLGSS.....TYQYNAKQL.VLSDQSVKTLASKGRLDPL.....QESMDYNN.
T.denticola/1-1395 VLYFKKIIRFSEIRSQREKIGKT.ISPYEDLSFRSYIK..ENLWKKTKNDEIGEKEFYD.
S.th_B/1-1121 KVVLQSVSPWRADVYFNKTTGKYEILGLKYADLQFEKGTGTYKISQEKYNDIKKKEGVD.
N.meningitidis/1-1082 TQQVKAV.....RVEQVQKTGVW.VRNHNGIADNATMVRVDVF.....EKGDKYY..
P.multocida/1-1056 QVKAIRV.....EQVQKSGVL.VRENNGVADNASIVRTDVF.....IKNNKFF..
C.jejuni/1-984 DFALKVLPNKAVARSKKGEIKDW.ILMDENYEFCFSLYKDSLILIQTKDMQEPEFVYYN.
A.naeslundii/1-1101 PVYAMLRVFTHDLLSQRHGDLFSAVIPPQSISMRCAEPKLRKA.....ITTGNATYLGW
PIM (CTD)
α54
α55
1270
1280
1290
1300
S.pyogenes/1-1368 .QHKHYLDEIIEQISEFS.....KRVILADAN....LDKVLSAYNKHRDKPIREQA
L.innocua/1-1334 .SNREMFAELLAHVSEFA.....KRYTLAEAN....LNKINQLFEQNKEGDIKAIA
S.mutans/1-1345 .KHKDEFKELLDVVSNFS.....KKYTLAEGN....LEKIKELYAQNNGEDLKELA
S.th_A/1-1388 .NHKKEFEELFYYILEFN.....ENYVGAKKN....GKLLNSAFQSWQNHSIDELC
F.novicida/1-1622 .AFDISKNEIVEAIIDSFTSKNIFWLPKNIELQKVDN...KNIFAIDTSKWFEVETPSDL
L.buchneri/1-1371 .....VYTEILDKVNQYF.....SLYDMNKF.....RHKLNLGFSKFISFPNHNVF
T.denticola/1-1395 .LLQKKNLEIYDMLLTKH.....KDTIYKKRPNSATIDILVKGKEKFKSLIIENQF
S.th_B/1-1121 .SDSEFKFTLYKNDLLLV.....KDTETKEQQL...FRFLSRTMPKQKHYVELKPY
N.meningitidis/1-1082 .LVPIYSWQVAKGILPDR.....AVVQGKDEED...WQLIDDSFNFKFSLHPNDLV
P.multocida/1-1056 .LVPIYTWQVAKGILPNK.....AIVAHKNEDE...WEEMDEGAKFKFSLFPNDLV
C.jejuni/1-984 .AFTSSTVSLIVSKHDNK.....FETLSKNQKILFKNANEKEV
A.naeslundii/1-1101 VVVGDELEINVDSFTKYA.....IGRFLEDFPNTTRWRIC..GYDTNSKLTLKPIV
PIM (CTD)
α56
η15
β25
β26
major groove
η16
1310
1320
1330
1340
S.pyogenes/1-1368 ENI.....IHLFTLTNLGAPAAFKYFD.....TTIDRKR.YTSTKEV.L
L.innocua/1-1334 QSF.....VDLMAFNAMGAPASFKFFE.....TTIERKR.YNNLKEL.L
S.mutans/1-1345 SSF.....INLLTFTAIGAPATFKFFD.....KNIDRKR.YTSTTEI.L
S.th_A/1-1388 SSF.....IGPTGSERKGLFELTSRGSAADFEFLG.....VKIPRYR.DYTPSSLL.K
F.novicida/1-1622 RDIGIATIQYKIDNNSRPKVRVKLDYVIDDDSKINYFMN....HSLLKSRYPDKVLEILK
L.buchneri/1-1371 DGN.....TKASSGKREILEEVLNGLHANPTFGNLKDIGITTPFGQLQPNGILLS.D
T.denticola/1-1395 EVI.....LEILKLFSATRNVSDLQHIGGSKYSGVAKIGNKISSL.D
S.th_B/1-1121 DKQ.....KFEGGEALIKVLGNVANSGQCKKGLGKSNISIYKVRTDVL...G
N.meningitidis/1-1082 EVI.....TKKARMFGYFASCHRGTGNINIRIHDLDHKIGKNGILEGIGV..K
P.multocida/1-1056 ELK.....TKKEYFFGYYIGLDRATGNISLKEHDGEISKGKDGVYRVGVKL..
C.jejuni/1-984 IAK.....SIGIQNLKVFEKYIVS..
A.naeslundii/1-1101 LAA.....EGLENPSSAVNEI.....VELKGWRVAINVLTK.V
PIM (CTD)
β27
β28
1350
1360
S.pyogenes/1-1368 DATLIHQSITG..LYETRIDLSQLGGD....
L.innocua/1-1334 NSTIIYQSITG..LYESRKRLDD.....
S.mutans/1-1345 NATLIHQSITG..LYETRIDLNKLGGD....
S.th_A/1-1388 DATLIHQSVTG..LYETRIDLAKLGEG....
F.novicida/1-1622 QSTIIEFESSG..FNKTIKEMLGMKLAGI..
L.buchneri/1-1371 EAKIRYQSPTG..LFERTVSLKDL.....
T.denticola/1-1395 NCILIYQSITG..IFEKRIDLLKV.....
S.th_B/1-1121 NQHIIKNEGDK.....PKLDF.....
N.meningitidis/1-1082 TALSFQKYQID..ELGKEIRPCRLKKRPPVR
P.multocida/1-1056 .ALSFEKYQVD..ELGKNRQICRPQQRQPVR
C.jejuni/1-984 ...ALGEVTKA..EFRQREDFKK.....
A.naeslundii/1-1101 HPTVVRRDALGRPRYSSRSNLPTSWTIE...