

[illegible]

Figure S1. Polymorphism of *N. gonorrhoeae mutS*. Analysis of the NEIS2138 locus revealed the presence of 342 allelic variants with 867 polymorphic sites for 2697 positions. Numbers of the first nucleotide in the rows are indicated above of the sequences. The percentage of alleles that have certain nucleotide substitution(s) at each position of the coding strand are shaded with different colors: from the smallest (pink) to the highest (black). See key above the figure. Deletions are indicated as “-”.

Key: 0-10 | >10-20 | >20-30 | >30-40 | >40-50 | >50-60 | >60-70 | >70-80 | >80-90 | >90-100

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1      10      20      30      40      50      60      70      80      90      100
ATGCCACGCATTGCCGCCCTGCCCGACCACTCGTCAACCAAAATGCCGCCGCGCAAGTGGTGAACGCCCTGCCAACGCCCTGAAAGAAATCGTTGAAA
      T T      T T      C T A A A A      T T C      C T A      C
101     110     120     130     140     150     160     170     180     190     200
ACAGCATAGACGCGGCGCAACGCGCGTTGATGTGGAAGTGAAGGCGCGGCATCCGCCCTC-----AT
      T C T A A A T G G A G      -C-G-      CG-----ATCCGCGTCGGCGACAACGCGCGGCATCCGCCCTC--
      - -G      CA      A C T G G      C
201     210     220     230     240     250     260     270     280     290     300
CCGCGTCGGCGCAACGCGCGGCATCCACCCGACGACATCGAACTCGCGCTCCACGCCACGCAACAGCAAAATCAAACCCCTGAACGATTGGAA
-----A--T--CT-----GG T      ATT A
TT      A      -T A-      -- A T      G
301     310     320     330     340     350     360     370     380     390     400
CAGCTTGCCAGCATGGGCTTTCCGCGCGAAGGCTTGGCCAGTATCGCCTCCGTCAGCCGCTGACCTGACCCGCGCAAGAAGACAGTTTCGCATCGCA
      T A      A T      A T A C      T G      CA ATT A      T      C -----C A
401     410     420     430     440     450     460     470     480     490     500
CCCAAGTCAAAGCGGAAGCGCAAACTCAGCAGCGCCACCGCGCGCCACCCCGTCGGCACCAACATCGAAGCGCGCAACTCTTCTTCAACACCCC
      C      A      AAA      TTG-T- A A      C T A T      A      T
      G      T
501     510     520     530     540     550     560     570     580     590     600
CGCGCGGCGCAAGTTCCCTCAAATCCGAAAACACCGAATACGCTCACTGCGCCACCATGCTCGAACGCCCTCGCGCTGGCGCATCCGCACATTGCCTTCTCA
T      A      A T      A      T C      A T      T      A T A      C      T      A G
601     610     620     630     640     650     660     670     680     690     700
CTCAAACGCGACGCGCAAACTGTTCAAATCTCTGCGCAAGCCCTGCAATGACGTCATCGCGCCATGTCGCGCATGATTTTCAGACGCGCATCTTTTGG
      A      CT AAT      T C      AG T      T      T AA
701     710     720     730     740     750     760     770     780     790     800
AAATTGACAGCGGCAATAGCGCGCTGCGGCTCTATGGCGCGATTGCGCAAGCCGACITTTGCGCCAAAGCGCAAAACCGGATAAACAATATTGCTTCGTCACCA
      G      AT A A      C      A AT      T      T C      C T      G
801     810     820     830     840     850     860     870     880     890     900
TCGTTTTCGCGGACAAAGTCATGCTCCATGCGCTCAAGCAGGCATACGCGACGATTTGCACACGCGCTTACGCGCTTTTCGTCCTTTTCCTCGAG
      T      G      C T      A T      T A      A      A G T      C T      C T      C
901     910     920     930     940     950     960     970     980     990     1000
CTGCCGCCGCAAGCCGTGGATGTCAACGCTCCACCCGACCAAAACCGAAATCCGCTTCCGCGCAGCGCGCAAGTACACCAACTCGTGTTCACACGCTCA
TA      A      C      A      T T A G G      T
1001    1010    1020    1030    1040    1050    1060    1070    1080    1090    1100
ACAAAGCCCTTGCCGACACACGCGCAACCTGACCGAAAGCGTCAGCAACGCGAGCGCAAGTGTTCATGACATTACCGCGCTTACGCTGCCCCAATGCC
      A      TA A G T T      T
      C
1101    1110    1120    1130    1140    1150    1160    1170    1180    1190    1200
GTCTGAAAACGACAGCGAAATCTGTTTATAGCGCATCCCAACCCGACAGGCAACAAACCCGATACACGCAATGCTTTGGTTTCATCAGGTAAAC
      C A      A C      A G T      T      G      G      C
1201    1210    1220    1230    1240    1250    1260    1270    1280    1290    1300
GCGCCCATGCCTTTACAGGCGCGCGTGGCGCGCAACACACAGCCTGTCCCTGCGCGAAAGCCGCGCGCAATGGACACCTATGCCGAACCTCTACAAA
      A G      T A      T      C A A      G A      T      A A C      A T G T      CA      G G
1301    1310    1320    1330    1340    1350    1360    1370    1380    1390    1400
AAACCGACGACATCGACCTTGAGTTGAGCCAAATTCGAACAGGCACGTTTCGGCAATATGCCGTCTGAAAACGCGTGCACAAACAGATACGCGCTTC
T TA      T      G G G      G      C      C      GCAGCA      GAC C      CG-----C
      A      C
1401    1410    1420    1430    1440    1450    1460    1470    1480    1490    1500
AGACGCGCATCCGCTCCCAATCGAACTGCCGCGCTCGGTTTCGCCATTGCCCAATTAAGTGGCATCTACATCTTTCGCCCAAGCGCAAGACAGCCTGTTG
      GGACAGGCT      A T A      A T      C T A      G
1501    1510    1520    1530    1540    1550    1560    1570    1580    1590    1600
CTCATCGATATGCACGCCGCTGCGAAGCGCTCAACTACGAGAAATGAAACGCCCAACGTCAGGAAAACGCGCAACCTGCAAGGCCAGCACCTGCTTATTC
      G      TAT TC      A      A      G      A A      A A      ATG
1601    1610    1620    1630    1640    1650    1660    1670    1680    1690    1700
CCGTAACTTTGCCGCGTCCACGAAGAATGCGCGCCCTCGCGCATCATGCCGAAACGCTGGCAGGCTTCGGGCTGGAAGTGTCCGACATGGGCGGCA
      C AA      A T      T--A-----A T G A A      -TT-----T---
      - - C      A--
1701    1710    1720    1730    1740    1750    1760    1770    1780    1790    1800
CACCCCTCGCGCTCCGCGCGCGCGCGTAATGTTGGGCAATCCGATGTCGTCTCCCTCGCACGCGACGTATTGGGCGCAACTCGCCCAAGTCGGCAGCAGC
T A T      A TT A CC AC A A      G      C      T A GT CAAA T      AAA      T      A A
      T G
1801    1810    1820    1830    1840    1850    1860    1870    1880    1890    1900
CAAACCATCGCATCACAGAAACCGCATCTCTGCCCAATGTCTCTGCCAGGCTCAATCCGCGCGCGCGCAGGCTCACCTGCGCCGAAATGAACGCGC
      A A GA      T      A G T      T -CT---C---T
      A- - -
1901    1910    1920    1930    1940    1950    1960    1970    1980    1990    2000
TGCTGCGCATATGGAATAACGCCGCGCAGCAACCAAGTGAACACGCGAGCGGCTGGGTCAAACCTGACTTTGAAAGAATTGGAACACACTGTTCTTT
T A      G      T      A      TT A G      T
2001    2010
GCGCGGACAGTAA
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Figure S2. Polymorphism of *N. gonorrhoeae* *mutL*. Analysis of the NEIS2138 locus revealed the presence of 310 variants with 460 polymorphic sites for 2017 positions. Numbers of the first nucleotide in the rows are indicated above of the sequences. The percentage of alleles that have certain nucleotide substitution(s) at each position of the coding strand are shaded with different colors: from the smallest (pink) to the highest (black). See key above the figure. Deletions are indicated as “-”.

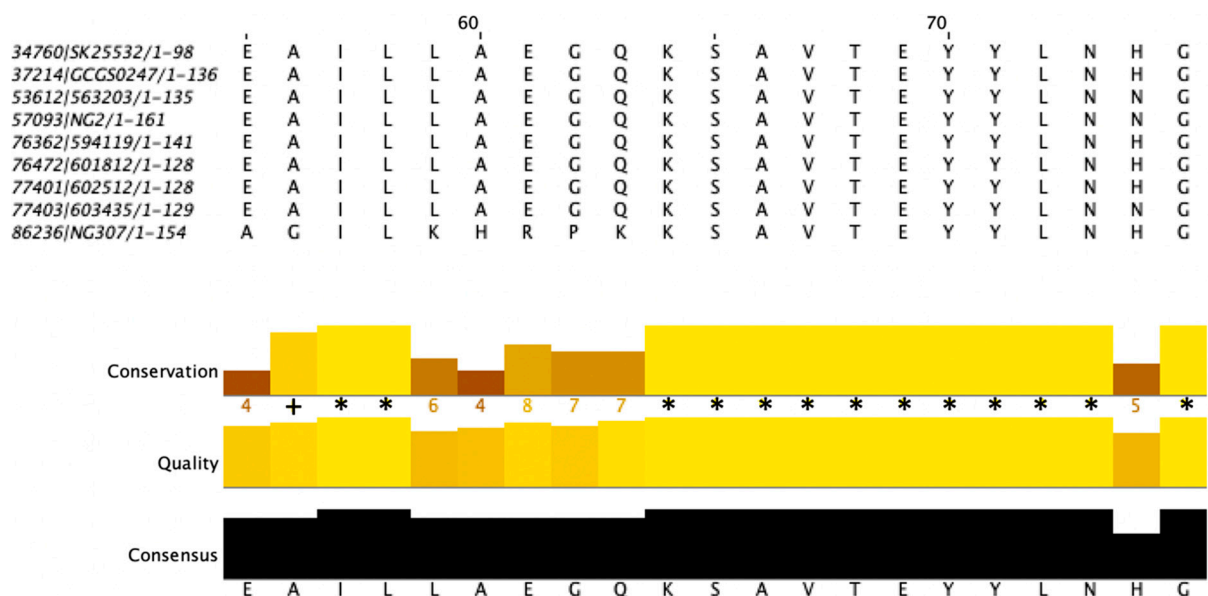


Figure S3. A part of an alignment of *N. gonorrhoeae* Pile amino acids from 3L group. The designations "*" correspond to completely conservative residues. The designations "+" indicate the small number of substitutions that do not affect the protein physico-chemical properties. Numerical indexes from 0 to 9 show the degree of identity in ascending order (0 corresponds to the most variable positions).

Me ²⁺	-	-	Mg ²⁺	Mn ²⁺	Ca ²⁺	Co ²⁺	Cd ²⁺	Zn ²⁺	Ni ²⁺
ngMutL/ngβ	-	+	+	+	+	+	+	+	+

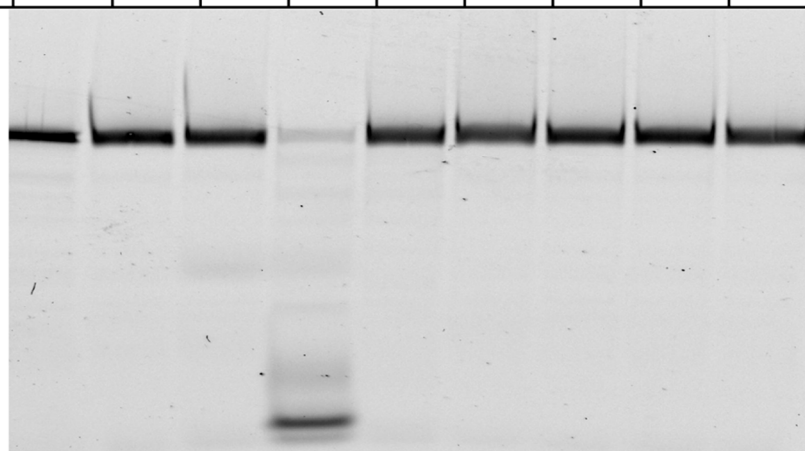


Figure S4. Effect of metal ions on ngMutL-induced hydrolysis of 76R/76M (10 nM). The reaction mixtures were incubated in the presence of 0.8 mM ATP, 5 mM metal ions (Mg^{2+} , Mn^{2+} , Ca^{2+} , Co^{2+} , Cd^{2+} , Zn^{2+} , Ni^{2+}) for 90 min at 37 °C, and then analyzed in a 12% polyacrylamide gel containing 7 M urea. 0.5 μM ngMutL (per dimer) was used in the presence of an equimolar amount of ng β dimer.

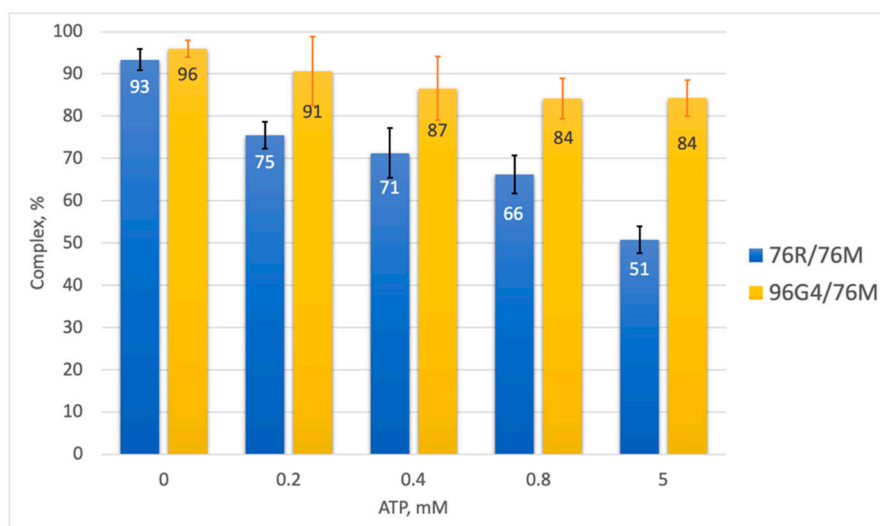


Figure S5. The effect of ATP on the ngMutL complex formation with 76R/76M (blue) and 95G4/76M (yellow) (20 nM concentration). The reaction mixtures (20 μ L) were incubated for 10 min on ice with 500 nM ngMutL (per dimer) in 20 mM HEPES buffer (pH 8.0) containing 100 mM KCl, 0.5 mg/mL BSA, 5 mM MgCl₂ and 1 mM DTT.

Samples were analyzed by electrophoresis in a 6% polyacrylamide gel in TAE buffer for 2–3 h at 4 °C.