

# Brenda Miner

## Annotations for ['1aja', '1ew2'] (3.1.3.1)

October 4, 2005

### 1 Downloads

#### 1.1 Structure-files

- 1aja.pdb from <http://projects.villa-bosch.de/dbase/pdba/mmol/1aja.pdb.gz>
- 1ew2.pdb from <http://projects.villa-bosch.de/dbase/pdba/mmol/1ew2.pdb.gz>

#### 1.2 Engineering

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| D101S | Escherichia coli | ['activity'] |

*Commentary:* weaker phosphate binding can be attributed to the increased flexibility of the Arg166 side chain, faster phosphate release is responsible for the 35fold higher activity

- | Name  | Organism         | Impact                   |
|-------|------------------|--------------------------|
| D153G | Escherichia coli | ['kinetics', 'activity'] |

*Commentary:* the mutant has 5fold higher catalytic activity but no change in  $K_m$  at pH 8.0 in 50 mM Tris-HCl. The mutation also affects  $Mg^{2+}$  binding, resulting in an enzyme with lower metal affinity. The mutation also affects the position of the water ligands of  $Mg^{2+}$  and the loop Gln152-Thr155 is shifted by 0.3 Å away from the active site. The weaker  $Mg^{2+}$  binding of the mutant compared with the wild type is caused by an altered coordination sphere in the proximity of the  $Mg^{2+}$  ion and also by the loss of an electrostatic interaction,  $Mg^{2+}/COO-Asp153$ , in the mutant

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| D153G | Escherichia coli | ['activity'] |

*Commentary:* weaker phosphate binding can be attributed to the increased flexibility of the Arg166 side chain, faster phosphate release is responsible for the 5fold higher activity, reduced magnesium affinity, maximal activity is only achieved with the addition of exogenous magnesium

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| D153H | Escherichia coli | ['activity'] |

*Commentary:* reduced magnesium affinity, maximal activity is only achieved with the addition of exogenous magnesium

- | Name        | Organism         | Impact       |
|-------------|------------------|--------------|
| D153H/K328A | Escherichia coli | ['activity'] |

*Commentary:* reduced magnesium affinity, maximal activity is only achieved with the addition of exogenous magnesium

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| D369A | Escherichia coli | ['kinetics'] |

*Commentary:* mutant enzyme shows reduced turnover rates and increased Km-value

- | Name  | Organism         | Impact                    |
|-------|------------------|---------------------------|
| D369N | Escherichia coli | ['kinetics', 'mechanism'] |

*Commentary:* mutant enzyme shows reduced turnover rates and increased Km-value. The reaction mechanism of the mutant enzyme involves only 1 metal with the possible assistance of a His side chain

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| D369N | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, highly reduced activity

- | Name  | Organism         | Impact                   |
|-------|------------------|--------------------------|
| D434E | Escherichia coli | ['kinetics', 'activity'] |

*Commentary:* site-directed mutagenesis, reduced activity, increased kcat and Km compared to the wild-type enzyme

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| E322K | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, highly reduced activity

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| E341K | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, highly reduced activity

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| H412Y | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, highly reduced activity

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| K328A | Escherichia coli | ['notclassified'] |

*Commentary:* lower phosphate affinity, alteration in the rate-limiting step

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| K328C | Escherichia coli | ['notclassified'] |

*Commentary:* lower phosphate affinity, alteration in the rate-limiting step

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| K328H | Escherichia coli | ['notclassified'] |

*Commentary:* lower phosphate affinity, alteration in the rate-limiting step

- | Name  | Organism     | Impact        |
|-------|--------------|---------------|
| R166A | Homo sapiens | ['mechanism'] |

*Commentary:* mutation changes the inhibition mechanism of the mutant enzyme to a more complex mixed-type inhibition with decreased affinities for L-Leu and L-Phe

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| R166A | Escherichia coli | ['notclassified'] |

*Commentary:* mutation has very little effect on turnover number, in presence of phosphate acceptor the substrate binding decreases over 50fold, phosphate inhibition is reduced 50fold

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| R166Q | Escherichia coli | ['notclassified'] |

*Commentary:* mutation has very little effect on turnover number, in presence of phosphate acceptor the substrate binding decreases over 50fold

- | Name  | Organism         | Impact            |
|-------|------------------|-------------------|
| R166S | Escherichia coli | ['notclassified'] |

*Commentary:* mutation has very little effect on turnover number, in presence of phosphate acceptor the substrate binding decreases over 50fold, phosphate inhibition is reduced 50fold

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| S102A | Escherichia coli | ['activity'] |

*Commentary:* activity is significantly less than that of the wild-type enzyme, but 100000-10000000fold greater than the non-enzymatic reaction, 1000-10000fold reduction in the turnover number

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| S102C | Escherichia coli | ['activity'] |

*Commentary:* activity is significantly less than that of the wild-type enzyme, but 100000-10000000fold greater than the non-enzymatic reaction, 100fold reduction in turnover number

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| S102G | Escherichia coli | ['activity'] |

*Commentary:* activity is significantly less than that of the wild-type enzyme, but 100000-10000000fold greater than the non-enzymatic reaction, 1000-10000fold reduction in the turnover number

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| S102L | Escherichia coli | ['activity'] |

*Commentary:* activity is significantly less than that of the wild-type enzyme, but 100000-10000000fold greater than the non-enzymatic reaction, 1000-10000fold reduction in the turnover number

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| S105L | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, reduced activity

- | Name  | Organism         | Impact       |
|-------|------------------|--------------|
| T155M | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, highly reduced activity

- | Name | Organism         | Impact       |
|------|------------------|--------------|
| T59A | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, exists as a dimer, shows catalytic activity and metal content similar to the wild-type enzyme

- | Name | Organism         | Impact       |
|------|------------------|--------------|
| T59R | Escherichia coli | ['activity'] |

*Commentary:* site-directed mutagenesis, exists as a monomer, shows 10000fold reduced activity compared to the wild-type, highly reduced metal content, highly reduced thermal stability

## 2 Alignment of Escherichia coli's Mutations

align to reference sequence:

Compare sequences of length 1 and 471

1	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
	-----
59	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
	-----
117	GCPNAAHDQKDISAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
	-----
175	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAQAQER
	-----
233	LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
	-----
291	YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
	-----
349	VGTSWATASAAASDTVYDPKGTCKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
	-----
407	ESDGMGDGILLIINKAPKDsLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
	-----
465	TRAKTVPTFLLPLLALAITSQM
	-----

minimal editing distance: 30 Alignment: -8

### 2.1 Align To Sequence In 1aja.pdb

Compare sequences of length 471 and 450

1	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ

```

117 GCPNAAXXXXXXXXSAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
117 GCPNAAHDQKDI SAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAEAQER
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAQAQER
233 LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233 LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
349 VGTSWATASAASTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
465 T-----
465 TRAKTVPTFLLPLLALAITSQKM

```

Matches with 94 **T59A** : 51 T  $\mapsto$  30 T  
**T59R** : 51 T  $\mapsto$  30 T  
Compare sequences of length 471 and 450

```

1 KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
1 KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSD EESNGYSMVMVAGD
59 KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
59 KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
117 GCPNAAXXXXXXXXSAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
117 GCPNAAHDQKDI SAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAEAQER
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAQAQER
233 LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233 LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
349 VGTSWATASAASTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
465 T-----
465 TRAKTVPTFLLPLLALAITSQKM

```

Matches with 93 **T59A** : 51 T  $\mapsto$  30 T  
**T59R** : 51 T  $\mapsto$  30 T

## 2.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 471 and 480

```

1 PPALDCATYPELC AAFAMVHAIF--TQE QVGHVLHAQP GRAFVAVDE--GAHTEED
1 K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
59 LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAKGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--

```

```

ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMR FMYKRGGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGR TTNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAAGA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLP LADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **T59A** : 51 T  $\mapsto$  31 T  
**T59R** : 51 T  $\mapsto$  31 T  
Compare sequences of length 471 and 480

```

PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAVAVDE--GAHTEED
1 K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
LPVASQQRYES-GSESETVDPRAGDKLVYGPNGYLLVY--AKRDRAGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD--PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMR FMYKRGGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGR TTNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAAGA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLP LADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **T59A** : 51 T  $\mapsto$  31 T  
**T59R** : 51 T  $\mapsto$  31 T

### 3 Alignment of Escherichia coli's Mutations

align to reference sequence:

Compare sequences of length 1 and 471

1	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
	-----
59	KTNLAQTLGPAKTDPAVIQSAHAHDATVIIVLTNGEKKAFELARQVAEDLDVTEGIQ
	-----
117	GCPNAAHDQKDISAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
	-----
175	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
	-----
233	LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
	-----
291	YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELiTPHDKEHIDVGLAGNYTK
	-----D-----
349	VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
	-----
407	ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
	-----
465	TRAKTVPTFLLPLLALAI TSQKM
	-----

minimal editing distance: 30 Alignment: -4

#### 3.1 Align To Sequence In 1aja.pdb

Compare sequences of length 471 and 450

1	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
	KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59	KTNLAQTLGPAKTDPAVIQSAHAHDATVIIVLTNGEKKAFELARQVAEDLDVTEGIQ
	KTNLAQTLGPAKTDPAVIQSAHAHDATVIIVLTNGEKKAFELARQVAEDLDVTEGIQ
117	GCPNAAXXXXXXXXSAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
	GCPNAAHDQKDISAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
175	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
233	LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
	LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
291	YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELiTPHDKEHIDVGLAGNYTK
	YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELiTPHDKEHIDVGLAGNYTK
349	VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
	VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
407	ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
	ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
465	T-----
	TRAKTVPTFLLPLLALAI TSQKM

Matches with 94 **D153G** : 149 D  $\leftrightarrow$  128 D

Compare sequences of length 471 and 450

```

1 KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXXYSMVMVAGD
KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59 KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
GCPNAXXXXXXXXXSAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
117 GCPNAAHDQKDISAGEVQLFFGKENKSLEIAKDTMQALTPVSDNRQPNPTCTVAP
KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233 LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTLPADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTLPADIGKFFGGAGEAYNRAATI
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
T-----
465 TRAKTVPTFLLPLLALAITSQKM

```

Matches with 93 D153G : 149 D  $\mapsto$  128 D

### 3.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 471 and 480

```

1 PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAVAVDE--GAHTEED
K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
59 LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAGPALGF
----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLQAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFRMYKRGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRRTNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLPADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE---AAERNWFDPNEEEE----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLALAITSQKM

```

Matches with 42 **D153G** : 149 D  $\mapsto$  121 C  
 Compare sequences of length 471 and 480

```

1  PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRFVAVDE--GAHTEED
K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
59  LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAKGPALGF
----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
117  ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
175  Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETMEMLSPDLTSD-RH-----
CPNAA--HDQKDISAGEVQLFFGKENKSLLLEIAKDTMQALTPV--SDNRQPNPTCT
----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233  VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFMYKRGGLIVDIDMN
291  YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349  L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407  NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465  DTVY-DPKGTKKNLA-YHTYQGTLPPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE----
523  GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMETRAKT
VPI-----I-----
581  VPTFLLPLLLALAITSQKM

```

Matches with 42 **D153G** : 149 D  $\mapsto$  121 C

## 4 Alignment of Escherichia coli's Mutations

align to reference sequence:

Compare sequences of length 228 and 471

```

1  KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
-----
59  KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
-----
117  GCPNAAHDQKDISAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
-----K????????????????????????????????????????????????????
175  KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
????????????????????????????????????????????????????????????
233  LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
????????????????????????????????????????????????????????????
291  YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
???R?????????????D?????????????????????????????????????????
349  VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTLPPLADIGKFFGGAGEAYNRAATI
????????????SD-----
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMET

```

```

407 -----
      TRAKTVPTFLLPLLLALAI TSQKM
465 -----

```

minimal editing distance: 300 Alignment: 21

#### 4.1 Align To Sequence In 1aja.pdb

Compare sequences of length 471 and 450

```

      KLGLAAKMTYFLD TQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXXYSMVMVAGD
1     KLGLAAKMTYFLD TQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
      KTNLAQTLGPAKTDP AVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
59    KTNLAQTLGPAKTDP AVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
      GCPNAAHXXXXXXXXSAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
117   GCPNAAHDKDISAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
      KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAEAQER
175   KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAEAQER
      LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233   LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
      YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291   YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
      VGTSWATASAA SDTVYDPKGT KKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
349   VGTSWATASAA SDTVYDPKGT KKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
      ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
407   ESDGMGDGILLIINKAPKDSLSDRLAATQDGT LRRAGGPATIDGQAARNELVPMEP
      T-----
465   TRAKTVPTFLLPLLLALAI TSQKM

```

Matches with 94 **D101S** : 122 D  $\mapsto$  101 D

- D153G** : 174 D  $\mapsto$  153 G
- D153H** : 174 D  $\mapsto$  153 G
- D153H/K328A** : 174 D  $\mapsto$  153 G
- K328A** : 349 K  $\mapsto$  328 X
- K328C** : 349 K  $\mapsto$  328 X
- K328H** : 349 K  $\mapsto$  328 X
- R166A** : 187 R  $\mapsto$  166 R
- R166Q** : 187 R  $\mapsto$  166 R
- R166S** : 187 R  $\mapsto$  166 R
- S102A** : 123 S  $\mapsto$  102 S
- S102C** : 123 S  $\mapsto$  102 S
- S102G** : 123 S  $\mapsto$  102 S
- S102L** : 123 S  $\mapsto$  102 S

Compare sequences of length 471 and 450

```

      KLGLAAKMTYFLD TQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXXYSMVMVAGD
1     KLGLAAKMTYFLD TQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
      KTNLAQTLGPAKTDP AVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
59    KTNLAQTLGPAKTDP AVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
      GCPNAXXXXXXXXXSAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP

```

```

117 GCPNAAHDQKDI SAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAEAQER
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLOYGRAQAQER
LTKGWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233 LTKGWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
T-----
465 TRAKTVPTFLLPLLLALAITSQKM

```

Matches with 93 **D101S** : 122 D → 101 D

**D153G** : 174 D → 153 G  
**D153H** : 174 D → 153 G  
**D153H/K328A** : 174 D → 153 G  
**K328A** : 349 K → 328 X  
**K328C** : 349 K → 328 X  
**K328H** : 349 K → 328 X  
**R166A** : 187 R → 166 R  
**R166Q** : 187 R → 166 R  
**R166S** : 187 R → 166 R  
**S102A** : 123 S → 102 S  
**S102C** : 123 S → 102 S  
**S102G** : 123 S → 102 S  
**S102L** : 123 S → 102 S

## 4.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 471 and 480

```

PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAFVAVDE--GAHTEED
1 K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAKGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFMYKRGGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRRVNT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRTTNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS

```

```

465 DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
DTVY-DPKGTKKNLA-YHTYQGTLPPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **D101S** : 122 D → 91 D

**D153G** : 174 D → 153 H  
**D153H** : 174 D → 153 H  
**D153H/K328A** : 174 D → 153 H  
**K328A** : 349 K → 317 H  
**K328C** : 349 K → 317 H  
**K328H** : 349 K → 317 H  
**R166A** : 187 R → 166 R  
**R166Q** : 187 R → 166 R  
**R166S** : 187 R → 166 R  
**S102A** : 123 S → 92 S  
**S102C** : 123 S → 92 S  
**S102G** : 123 S → 92 S  
**S102L** : 123 S → 92 S

Compare sequences of length 471 and 480

```

1 PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAVAVDE--GAHTEED
K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAKGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFF--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLLRLAAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPV--SDNRQPNPTCT
----IE--Y--K-----MDGPEFLGMLH-----TVSPDLQAQMLETRNVV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFRMYKRGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD--ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
GVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLPPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **D101S** : 122 D → 91 D

**D153G** : 174 D → 153 H  
**D153H** : 174 D → 153 H  
**D153H/K328A** : 174 D → 153 H

**K328A** : 349 K  $\mapsto$  317 H  
**K328C** : 349 K  $\mapsto$  317 H  
**K328H** : 349 K  $\mapsto$  317 H  
**R166A** : 187 R  $\mapsto$  166 R  
**R166Q** : 187 R  $\mapsto$  166 R  
**R166S** : 187 R  $\mapsto$  166 R  
**S102A** : 123 S  $\mapsto$  92 S  
**S102C** : 123 S  $\mapsto$  92 S  
**S102G** : 123 S  $\mapsto$  92 S  
**S102L** : 123 S  $\mapsto$  92 S

## 5 Alignment of Escherichia coli's Mutations

align to reference sequence:

Compare sequences of length 1 and 471

1	KLGLAAKMTYFLDTQDTLGVVNAAHHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
	-----
	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVaEDLDVTEGIQ
59	-----D-----
	GCPNAAHDQKDISAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
117	-----
	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAQAQER
175	-----
	LTKGQWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233	-----
	YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291	-----
	VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
349	-----
	ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407	-----
	TRAKTVPTFLLPLLALAITSQKM
465	-----

minimal editing distance: 30 Alignment: -2

### 5.1 Align To Sequence In 1aja.pdb

Compare sequences of length 471 and 450

1	KLGLAAKMTYFLDTQDTLGVVNAAHHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
	KLGLAAKMTYFLDTQDTLGVVNAAHHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
	KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
117	GCPNAAXXXXXXXXSAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
	GCPNAAHDQKDISAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
175	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAEAQER
	KDINGHYTAKPGLWRVPMNGDAFLGLLPKQQAETVSNLSAADSVLQYGRAQAQER

```

233 LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
YCKRSTVHAVLAAPTAGQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
T-----
465 TRAKTVPTFLLPLLALAITSQKM

```

Matches with 94 **D369A** : 367 D  $\mapsto$  346 D  
**D369N** : 367 D  $\mapsto$  346 D  
Compare sequences of length 471 and 450

```

1 KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59 KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
GCPNAXXXXXXXXXSAGEVQLFFGKENKSILLEIAKDTMQALTPVSDNRQPNPTCTVAP
117 GCPNAAHDQKDISAGEVQLFFGKENKSILLEIAKDTMQALTPVSDNRQPNPTCTVAP
KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
175 KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233 LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
YCKRSTVHAVLAAPTAGQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291 YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
349 VGTSWATASAASDTVYDPKGTKKNLAYHTYQGTPLADIGKFFGGAGEAYNRAATI
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407 ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
T-----
465 TRAKTVPTFLLPLLALAITSQKM

```

Matches with 93 **D369A** : 367 D  $\mapsto$  346 D  
**D369N** : 367 D  $\mapsto$  346 D

## 5.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 471 and 480

```

1 PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRFVAVDE--GAHTEED
K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
59 LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVY--AKRDRAKGPALGF
----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSILLEIAKDTMQALTPV--SDNRQPNPTCT

```

```

-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFRMYKRGGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAAGA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **D369A** : 367 D  $\mapsto$  336 D  
**D369N** : 367 D  $\mapsto$  336 D  
Compare sequences of length 471 and 480

```

PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAVAVDE--GAHTEED
1 K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVY--AKRDRAKGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLLRLAETMEMLSPLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLSAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFRMYKRGGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAAGA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMEPTRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 **D369A** : 367 D  $\mapsto$  336 D  
**D369N** : 367 D  $\mapsto$  336 D

## 6 Alignment of Escherichia coli's Mutations

align to reference sequence:

Compare sequences of length 330 and 471

```

1  KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
-----D????????????????????????????????H????????????????????
59  KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
????????????????????????????????D????????????????????????????E???
117  GCPNAAHDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
????????????????????E????????????????????????????????????????
175  KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
????????????????????????????????????????????????????????????
233  LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
????????????????????????????????????????????????????????????
YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291  ?????????????????T????????????????????????????????????????
VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPPLADIGKFFGGAGEAYNRAATI
349  ?????????S-----
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407  -----
TRAKTVPTFLLPLLALAITSQKM
465  -----

```

minimal editing distance: 300 Alignment: 21

### 6.1 Align To Sequence In 1aja.pdb

Compare sequences of length 471 and 450

```

1  KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXYSMVMVAGD
KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
59  KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
117  GCPNAAHXXXXXXXXSAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
GCPNAAHDQKDISAGEVQLFFGKENKSLLEIAKDTMQALTPVSDNRQPNPTCTVAP
175  KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAQAQER
233  LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
LTKGWEGATATEAF TKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291  YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPPLADIGKFFGGAGEAYNRAATI
349  VGTSWATASAASDTVYDPKGTCKKNLAYHTYQGTLPPLADIGKFFGGAGEAYNRAATI
ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407  ESDGMGDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
T-----
465  TRAKTVPTFLLPLLALAITSQKM

```

Matches with 94 **D369N** : 390 D  $\mapsto$  369 D  
**D434E** : 455 D  $\mapsto$  434 D  
**E322K** : 343 E  $\mapsto$  322 E  
**E341K** : 362 E  $\mapsto$  341 E

**H412Y** : 433 H  $\mapsto$  412 H  
**S105L** : 126 S  $\mapsto$  105 S  
**T155M** : 176 T  $\mapsto$  155 T  
 Compare sequences of length 471 and 450

```

1  KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEXXXXXXXXXXYSMVMVAGD
59  KLGLAAKMTYFLDTQDTLGVVNAAHPGYAAIRLQSGTHEQSDEESNGYSMVMVAGD
   KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
177  KTNLAQTLGPAKTDPAVIQSAHAHDATVIVLTNGEKKAFELARQVAEDLDVTEGIQ
   GCPNAXXXXXXXXXSAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
187  GCPNAAHDQKDI SAGEVQLFFGKENKSLLLEIAKDTMQALTPVSDNRQPNPTCTVAP
   KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
175  KDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSNLSAADSVLQYGRAEAQER
   LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
233  LTKGQWEGATATEAFTKAGGGLTVDARANLLQETISGKGGKELANGPCKESTASPG
   YCKRSTVHAVLAAPTAGQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
291  YCKRSTVHAVLAAPTADQLEATSVNGTALGAAKAMELITPHDKEHIDVGLAGNYTK
   VGTSWATASAASDTVYDPKGTTKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
349  VGTSWATASAASDTVYDPKGTTKKNLAYHTYQGTLPLADIGKFFGGAGEAYNRAATI
   ESDGMDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
407  ESDGMDGILLIINKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAARNELVPMEP
   T-----
465  TRAKTVPTFLLPLLALAITSQKM
  
```

Matches with 93 **D369N** : 390 D  $\mapsto$  369 D  
**D434E** : 455 D  $\mapsto$  434 D  
**E322K** : 343 E  $\mapsto$  322 E  
**E341K** : 362 E  $\mapsto$  341 E  
**H412Y** : 433 H  $\mapsto$  412 H  
**S105L** : 126 S  $\mapsto$  105 S  
**T155M** : 176 T  $\mapsto$  155 T

## 6.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 471 and 480

```

1  PPALDCATYPELCAAFAMVHAIF--TQEQVGHVLHAQPGRAFVAVDE--GAHTEED
   K--LG-----L-AAK-MTY--FLDTQDTLGVVNAAHPGYA--AIRLQSGTH-EQ-
59  LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTY--AKRDRAGPALGF
   ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
   ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117  IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
   Y--ARSEHHGHDIRGGEVFLFFGRPNRSLRLAETMEMLSPDLTSD-RH-----
175  CPNAA--HDQKDISAGEVQLFFGKENKSLLLEIAKDTMQALTPV--SDNRQPNPTCT
   ----IE--Y--K-----MDGPEFLGMLH-----TVSPDLQAQMLETRNVV--
233  VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQONAETVSN-LSAADS-----VLQ
   Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP--TGMRFMYKRGGLIVDIDMN
291  YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
   SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
  
```

```

349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLPPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMETRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 D369N : 390 D → 357 D

D434E : 455 D → 454 E  
E322K : 343 E → 311 E  
E341K : 362 E → 330 E  
H412Y : 433 H → 432 H  
S105L : 126 S → 95 T  
T155M : 176 T → 155 S

Compare sequences of length 471 and 480

```

PPALDCATYPELCAAFAMVHAIF--TQEQVGHVHLHAQPGRFVAVDE--GAHTEED
1 K--LG-----L-AAK-MTY--FLDQTDLGVVNAAHPGYA--AIRLQSGTH-EQ-
LPVASQQRYEPS-GSESETVDPRAGDKLVYGPNGYLLVTVY--AKRDRAGPALGF
59 ----SDE--E-SNGY-SM-VMV-AGDKT-----N--LAQTLGPAKTD----PAV--
ISSGRLPYGGFSFVHSHDATVLSLTD-E----ESTLQGAREIA-D-DFMITETLAR
117 IQSA-----HAHDATVIVLTNGEKKAFE--L--ARQVAEDLDV--TEGIQG
Y--ARSEHHGHDIRGGEVFLFFGRPNRSLLRLAAETMEMLSPDLTSD-RH-----
175 CPNAA--HDQKDISAGEVQLFFGKENSLLLEIAKDTMQALTPV--SDNRQPNPTCT
-----IE--Y--K-----MDGPEFLGMLH-----TVSPDLQAQMLETRNWV--
233 VAPKDINGHYTAKPGLWRVPMNGDAFLGLLPKQQNAETVSN-LSAADS-----VLQ
Y-RAGQRKALWEQVLNKGDLRTGGQSYDDPYEPDP-TGMRFMYKRGGLIVDIDMN
291 YGRA-Q--AQ-ER-LTKG-----QW-----EGATATEA-FT-KAGGGLTVDARAN
SILQ-TAIDQCG--EQRASAPVD---ADS--YWNRNVT-HAYTGAPSAHQVRTTTV
349 L-LQET-ISGKGGKEL-ANGPCKESTA-SPGYCKRS-TVHAVLAAPTADQLEATSV
VGVSKGAKKARNMVSIVENGRITNCQNFRAAASL-GI-TQFNGKVGCLYATATAGS
407 NGTALGAACA--MELI-----TPHDKEHIDVG-LAGNYT----KVGTSWATASAAS
DPVHKDVNYTKS-LAVYPFRDMALP---IEPGLKDKKQ-GKLI-RAATVTSVGMGD
465 DTVY-DPKGTKKNLA-YHTYQGTLPPLADI--G-KFFGGAGEAYNRAATIESDGMGD
G-LFIILNKA-----A-TQAPQLKKAAGLAE----AAERNWFDPNEEE-----
523 GILLII-NKAPKDSLSDRLAATQDGTLLRRAGGPATIDGQAA-RNELVPMETRAKT
VPI-----I-----
581 VPTFLLPLLLALAITSQKM

```

Matches with 42 D369N : 390 D → 357 D

D434E : 455 D → 454 E  
E322K : 343 E → 311 E  
E341K : 362 E → 330 E  
H412Y : 433 H → 432 H  
S105L : 126 S → 95 T  
T155M : 176 T → 155 S

## 7 Alignment of Homo sapiens's Mutations

align to reference sequence:

Compare sequences of length 1 and 535

1	PATATELLLLLTGALLPLLAPVVS	RGPHAADTTGAPPALDCATYPELCAAFAMVHAI						
59	FTQE	QVGHVLHAQPGRA	FVAVDEGAHTEEDLPVASQQR	YEP	SGSESETVDPRAGDK			
117	LVYGP	NGYLLV	TYAKRDR	AKG	PALGF	ISSGRLPYGGF	SFVHSHDATVLSLTDEES	
175	TLQ	GAREI	ADDFMITETL	ARYAR	SEHHGHDIRGGEV	FLFFGRPNRSLRLAAETME		
233	MLSPDLT	SDRHIEYKMDGPE	FLGMLHTVSP	DL	SAQMLETRN	WVYRAGQRKALWEQV		
291	LNK	GDLRTGGQ	SYDDPYEPDPT	GMR	FM	YKRGGGLIVDIDMNSILQTAIDQCGEQRA		
349	SAPVD	ADSYWNRNV	THAYTGAPSAHQ	VRTTTTV	v	G	VSKGAKKARNMVSIVENGR	TTN
407	CQN	FRAAASL	GITQFNGK	VGCLYATATAGSD	PVHKDVNYTKSLAVYP	FRDMALPIE		
465	PGLK	DKKQ	KLIRAA	TVTSVGM	GDGLFII	LNKAATQAPQLKKAAGLAEAAERNWFD		
523	PNEEE	VPIIGLSL	QLRLGL	LLLLLLLLLMCPGLM				

minimal editing distance: 30 Alignment: -10

### 7.1 Align To Sequence In 1aja.pdb

Compare sequences of length 535 and 450

1	K----	L----	G-L----	A-----	AKMTYF----	LD--	TQDTL	GVVNA---	A-
59	PATATE	LLLLT	GALLP	LLAPV	VSRG	PHAADTTGAPPALDCATYPELCAAFAMVHAI			
117	FTQE	QVGHVLHAQPGRA	FVAVDE--	GAHTEEDLPVASQQR	YEP	SGSESETVDPRAGDKT			
175	DKT	-----	H-----	PGYA--	AIRLQSGTH-EXXXXXXXX--	Y--SMVM---V---AG			
233	DKL	VYGPNGYLLV	TY--	AKRDR	AKG	PALGF	ISSGRLPYGGF	SFVHSHDATVLSLT	
291	NKE	KAFE--	L--	ARQVAEDLDV--	TEGIQ	GPCNAAXXXXXXSA-G-EVQLFFGKE			
349	D-E	----	ESTLQ	GAREIA-D-DFMITETL	ARY--	ARSEHHGHDIRGGEVFLFFGRPNKSLLEIAKDTMQUALTPV--SDNRQPNPTCTVAPKDINGHYTAKPGLWRVPMNGDANRSLRLAAETMEMLSPDLTSD-RH-----IE--Y--K-----MDGPEFLGLLPKQQNAETVSN-LSAADS-----VLQY--G-R-A--EAQER----L-TKGQFLGMLH-----TVSPDL			
407	W----	EGATATEA-FT-KAGGGLTVDARANL-LQET-ISGKGGKEL-ANGPCKES							
465	SYDDPYEPDP-TGMR	FM	YKRGGGLIVDIDMNSILQ-TAIDQC	G--	EQRASAPVD--TA-SPGYCKRSTV-HAVLAAPTAGQLEATSVNGTALGAACA--MELI-----TPHD-ADS--YWNRN-VTHAYTGAPSAHQVRTTTTVVGVSKGAKKARNMVSIVENGR				

```

LADI--G-KFFGGAGEAYNRAATIESDGMGDGILLII-NKA----PKDSLSDRLAA
523 ---IEPGLKDKKQ-GKLI-RAATVTSVGMGDG-LFIILNKAATQAPQ--LKK--AA
TQDGTLLRRAGG-----PAT----IDG---QAARNELVP----MEPT--
581 ---G-LAEAAERNWFDPNNEEVP IIGLSLQL-RLGLLLLLLLLMCPGLM

```

Matches with 40 **R166A** : 156 R  $\mapsto$  0 -  
Compare sequences of length 535 and 450

```

K-----L-----G-L-----A-----AKMTYF-----LD--TQDTLGVVNA---A-
1 PATATELLLLLTGALLPLLAPVVSRRGPHAADTTGAPPALDCATYPELCAAFAMVHAI
-----H-----PGYA--AIRLQSGTH-EXXXXXXXXX--Y--SMVM---V---AG
59 FTQEQVGHVHLHAQPGRAFVAVDE--GAHTEEDLPVASQQRYEPSGSESETVDPRAG
DKT-----N--LAQTLGPAKTD---PAV--IQSA-----HAHDATVIVLT
117 DKLVYGPNGYLLVITY--AKRDRAKGPALGFISGRLPYGGFSFVHSHDATVLSLT
NGEKKAFE--L--ARQVAEDLDV--TEGIQGCNAXXXXXXXXXSA-G-EVQLFFGKE
175 D-E---ESTLQGAREIA-D-DFMITETLARY--ARSEHHGHDIRGGEVFLFFGRP
NKSILLEIAKDTMQALTPV--SDNRQPNPTCTVAPKDIINGHYTAKPGLWRVPMNGDA
233 NRSLLRLAAETMEMLSPDLTSD-RH-----IE--Y--K-----MDGPE
FLGLLPKQONAETVSN-LSAADS-----VLQY--G-R-A--EAQER----L-TKGQ
291 FLGMLH-----TVSPDLAQMLETRNWV--YRAGQRKALWE-QVLNKGDLRTGGQ
W-----EGATATEA-FT-KAGGGLTVDARANL-LQET-ISGKGGKEL-ANGPCKES
349 SYDDPYEPDP-TGMRFRMYKRGGGLIVDIDMNSILQ-TAIDQCG--EQRASAPVD--
TA-SPGYCKRSTV-HAVLAAPTAGQLEATSVNGTALGAACA--MELI-----TPHD
407 -ADS--YWNRN-VTHAYTGAPSAHQVRTTTVVGVSKGAKKARNMVSIVENGRTTNC
KEHIDVG-LAGNYT----KVGTSWATASASADTVY-DPKGTKNLA-YHTYQGTLP
465 QNFRAAASL-GI-TQFNGKVGCLYATATAGSDPVHKDVNYTKS-LAVYFPRDMALP
LADI--G-KFFGGAGEAYNRAATIESDGMGDGILLII-NKA----PKDSLSDRLAA
523 ---IEPGLKDKKQ-GKLI-RAATVTSVGMGDG-LFIILNKAATQAPQ--LKK--AA
TQDGTLLRRAGG-----PAT----IDG---QAARNELVP----MEPT--
581 ---G-LAEAAERNWFDPNNEEVP IIGLSLQL-RLGLLLLLLLLMCPGLM

```

Matches with 40 **R166A** : 156 R  $\mapsto$  0 -

## 7.2 Align To Sequence In 1ew2.pdb

Compare sequences of length 535 and 480

```

P-----P--A-----LDATYPELCAAFAMVHAI
1 PATATELLLLLTGALLPLLAPVVSRRGPHAADTTGAPPALDCATYPELCAAFAMVHAI
FTQEQVGHVHLHAQPGRAFVAVDEGAHTEEDLPVASQQRYEPSGSESETVDPRAGDK
59 FTQEQVGHVHLHAQPGRAFVAVDEGAHTEEDLPVASQQRYEPSGSESETVDPRAGDK
LVYGPNGYLLVITYAKRDRAKGPALGFISGRLPYGGFSFVHSHDATVLSLTDEES
117 LVYGPNGYLLVITYAKRDRAKGPALGFISGRLPYGGFSFVHSHDATVLSLTDEES
TLQGAREIADDFMITETLARYARSEHHGHDIRGGEVFLFFGRPNRSLLRLAAETME
175 TLQGAREIADDFMITETLARYARSEHHGHDIRGGEVFLFFGRPNRSLLRLAAETME
MLSPDLTSDRHIEYKMDGPEFLGMLHTVSPDLAQMLETRNWVYRAGQRKALWEQV
233 MLSPDLTSDRHIEYKMDGPEFLGMLHTVSPDLAQMLETRNWVYRAGQRKALWEQV
LNKGDRLRTGGQSYDDPYEPDPTGMRFRMYKRGGGLIVDIDMNSILQTAIDQCGEQRA
291 LNKGDRLRTGGQSYDDPYEPDPTGMRFRMYKRGGGLIVDIDMNSILQTAIDQCGEQRA

```

```

349 SAPVDADSYWNRNVTHAYTGAPSAHQVRTTTTVVGVSKGAKKARNMVSIVENGRITN
CQNFRAAASLGITQFNGKVGCLYATATAGSDPVHKDVNYTKSLAVYPFRDMALPIE
407 CQNFRAAASLGITQFNGKVGCLYATATAGSDPVHKDVNYTKSLAVYPFRDMALPIE
PGLKDKKQGKLIRAAATVTSVGMGDGLFIIILNKAATQAPQLKKAAGLAEAAAERNWFD
465 PGLKDKKQGKLIRAAATVTSVGMGDGLFIIILNKAATQAPQLKKAAGLAEAAAERNWFD
PNEEEVPII-----
523 PNEEEVPIIIGLSLQLRLGLLLLLLLLLMCPGLM

```

Matches with 94 **R166A** : 156 R  $\mapsto$  135 R  
Compare sequences of length 535 and 480

```

P-----P--A-----LDCATYPELCAAFAMVHAI
1 PATATELLLLLTGALLPLLAPVVSRRGPHAADTTGAPPALDCATYPELCAAFAMVHAI
FTQEQVGHVHLHAQPGRFVAVDEGAHTEEDLPVASQORYEPSGSESETVDPRAGDK
59 FTQEQVGHVHLHAQPGRFVAVDEGAHTEEDLPVASQORYEPSGSESETVDPRAGDK
LVYGPNGYLLVITYAKRDRAKGPALGFISGRLPYGGFSFVHSHDATVLSLTDEES
117 LVYGPNGYLLVITYAKRDRAKGPALGFISGRLPYGGFSFVHSHDATVLSLTDEES
TLQGAREIADDFMITETLARYARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETME
175 TLQGAREIADDFMITETLARYARSEHHGHDIRGGEVFLFFGRPNRSLRLAAETME
MLSPDLTSDRHIEYKMDGPEFLGMLHTVSPDLAQMLETRNWVYRAGQRKALWEQV
233 MLSPDLTSDRHIEYKMDGPEFLGMLHTVSPDLAQMLETRNWVYRAGQRKALWEQV
LNKGLRGTGGQSYDDPYEPDPTGMRFRMYKRGGLIVDIDMNSILQTAIDQCCEQRA
291 LNKGLRGTGGQSYDDPYEPDPTGMRFRMYKRGGLIVDIDMNSILQTAIDQCCEQRA
SAPVDADSYWNRNVTHAYTGAPSAHQVRTTTTVVGVSKGAKKARNMVSIVENGRITN
349 SAPVDADSYWNRNVTHAYTGAPSAHQVRTTTTVVGVSKGAKKARNMVSIVENGRITN
CQNFRAAASLGITQFNGKVGCLYATATAGSDPVHKDVNYTKSLAVYPFRDMALPIE
407 CQNFRAAASLGITQFNGKVGCLYATATAGSDPVHKDVNYTKSLAVYPFRDMALPIE
PGLKDKKQGKLIRAAATVTSVGMGDGLFIIILNKAATQAPQLKKAAGLAEAAAERNWFD
465 PGLKDKKQGKLIRAAATVTSVGMGDGLFIIILNKAATQAPQLKKAAGLAEAAAERNWFD
PNEEEVPII-----
523 PNEEEVPIIIGLSLQLRLGLLLLLLLLLMCPGLM

```

Matches with 94 **R166A** : 156 R  $\mapsto$  135 R