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Annotations for ['1ejj', '1e58'] (5.4.2.1)

October 4, 2005

1 Downloads

1.1 Structure-files

- 1ejj.pdb from <http://projects.villa-bosch.de/dbase/pdba/mmol/1ejj.pdb.gz>
- 1e58.pdb from <http://projects.villa-bosch.de/dbase/pdba/mmol/1e58.pdb.gz>

1.2 Engineering

- | Name | Organism | Impact |
|------|--------------------------|--------------|
| A60S | Saccharomyces cerevisiae | ['activity'] |

Commentary: 69

- | Name | Organism | Impact |
|------|-----------------------------|--------------|
| D12N | Bacillus stearothermophilus | ['activity'] |

Commentary: no activity

- | Name | Organism | Impact |
|------|--------------------------|--------------|
| E86Q | Saccharomyces cerevisiae | ['activity'] |

Commentary: 1

- | Name | Organism | Impact |
|------|---------------------------|--------------|
| E93D | Schizosaccharomyces pombe | ['activity'] |

Commentary: less than 1

- | Name | Organism | Impact |
|------|---------------------------|-------------------|
| E93D | Schizosaccharomyces pombe | ['notclassified'] |

Commentary: 3D structure in solution obtained with NMR

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H123N | Bacillus stearothermophilus | ['activity'] |

Commentary: 3

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H125N | Bacillus stearothermophilus | ['activity'] |

Commentary: 67

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H128N | Bacillus stearothermophilus | ['activity'] |

Commentary: 20

- | Name | Organism | Impact |
|-------|--------------------------|--------------|
| H181A | Saccharomyces cerevisiae | ['activity'] |

Commentary: His181 is substituted by Ala in site-directed mutagenesis. The resulting enzyme has a reduced activity and still requires 2,3-diphosphoglycerate. His181 seems to be important for cofactor-binding

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H407N | Bacillus stearothermophilus | ['activity'] |

Commentary: no activity

- | Name | Organism | Impact |
|------|-----------------------------|--------------|
| H42N | Bacillus stearothermophilus | ['activity'] |

Commentary: 91

- | Name | Organism | Impact |
|------------|-----------------------------|--------------|
| H42N/H128N | Bacillus stearothermophilus | ['activity'] |

Commentary: 8

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H445N | Bacillus stearothermophilus | ['activity'] |

Commentary: 18

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| H462N | Bacillus stearothermophilus | ['activity'] |

Commentary: 0.3

- | Name | Organism | Impact |
|------|-----------------------------|--------------|
| H66N | Bacillus stearothermophilus | ['activity'] |

Commentary: 2

- | Name | Organism | Impact |
|-------|--------------------------|---------------|
| K246G | Saccharomyces cerevisiae | ['mechanism'] |

Commentary: mutant enzymes in which Ser11 is replaced by Gly, i.e. S11G and Lys246 by Gly, i.e. K246G do not have significantly altered kinetic values

- | Name | Organism | Impact |
|-------|--------------------------|--------------|
| L245G | Saccharomyces cerevisiae | ['activity'] |

Commentary: 39

- | Name | Organism | Impact |
|-------------|--------------------------|--------------|
| L245G/L246G | Saccharomyces cerevisiae | ['activity'] |

Commentary: 105

- | Name | Organism | Impact |
|-------|--------------------------|--------------|
| L246G | Saccharomyces cerevisiae | ['activity'] |

Commentary: 98

- | Name | Organism | Impact |
|-------|---------------------------|--------------|
| R120Q | Schizosaccharomyces pombe | ['activity'] |

Commentary: 59

- | Name | Organism | Impact |
|-------------|---------------------------|--------------|
| R120Q/R121Q | Schizosaccharomyces pombe | ['activity'] |

Commentary: 62

- | Name | Organism | Impact |
|-------|---------------------------|--------------|
| R121Q | Schizosaccharomyces pombe | ['activity'] |

Commentary: 12

- | Name | Organism | Impact |
|------|---------------------------|--------------|
| R14Q | Schizosaccharomyces pombe | ['activity'] |

Commentary: less than 1

- | Name | Organism | Impact |
|-------|-----------------------------|--------------|
| R261L | Bacillus stearothermophilus | ['activity'] |

Commentary: no activity

- | Name | Organism | Impact |
|------|---------------------------|--------------|
| R94Q | Schizosaccharomyces pombe | ['activity'] |

Commentary: 1

- | Name | Organism | Impact |
|------|--------------------------|--------------|
| S11A | Saccharomyces cerevisiae | ['activity'] |

Commentary: 4

- | Name | Organism | Impact |
|------|--------------------------|---------------|
| S11G | Saccharomyces cerevisiae | ['mechanism'] |

Commentary: mutant enzymes in which Ser11 is replaced by Gly, i.e. S11G and Lys246 by Gly, i.e. K246G do not have significantly altered kinetic values

- | Name | Organism | Impact |
|------|---------------------------|--------------|
| S62A | Schizosaccharomyces pombe | ['activity'] |

Commentary: loss of activity during purification

- | Name | Organism | Impact |
|------|-----------------------------|--------------|
| S62A | Bacillus stearothermophilus | ['activity'] |

Commentary: no activity

- | Name | Organism | Impact |
|------|-----------------------------|--------------|
| S62A | Bacillus stearothermophilus | ['activity'] |

Commentary: no phosphoglycerate mutase activity

2 Alignment of Bacillus stearothermophilus's Mutations

align to reference sequence:

Compare sequences of length 1 and 510

1	KVILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLKIGKKTIVIVPVPNTTHATQPKG

	DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
59	-----
	YNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFKEERGGSM
117	-----
	FFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGKVTESFHTLCVFFLHK
175	-----
	PHKGRDFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPRGDERVIVSPLVF
233	-----
	EDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMSYYRGSLSLTAIEGV
291	-----
	GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSVGG
349	-----
	DSLLGFLHLSLSTGHQVHNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGv
407	-----
	ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGDLIIL
465	-S-----
	AVPKKS
523	-----

minimal editing distance: 30 Alignment: -2

2.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 510 and 511

	-VILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLKIGKKTIVIVPVPNTTHATQPKG
1	KVILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLKIGKKTIVIVPVPNTTHATQPKG
	DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
59	DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
	YNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFEEERGGSM
117	YNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFKEERGGSM
	FFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGAVTESFHTLCVFFLHK
175	FFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGKVTESFHTLCVFFLHK
	PHKGRDFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPRGDERVIVSPLVF
233	PHKGRDFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPRGDERVIVSPLVF
	EDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMSYYRGSLSLTAIEGV
291	EDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMSYYRGSLSLTAIEGV
	GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSVGG
349	GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSVGG
	DSLLGFLHLSLSTGHQVHNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGv
407	DSLLGFLHLSLSTGHQVHNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGv
	ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGDLIIL

```

465 ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGDLIIL
AVPKKXX-
523 AVPKKS--

```

Matches with 99 **S62A** : 60 S \mapsto 62 S

2.2 Align To Sequence In 1e58.pdb

Compare sequences of length 510 and 248

```

K-----G-----QN-----A-----VAA-----A---KA
1 KVILSKGTMEKPPQLGLLDLMTPALDGLIGGDRLKIGKKTIVIVPVPNTTHATQPKG
AI---EDANGLYYR-----K-LP---KFN-EDF-EYVL---PV---GT-----PI
59 DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAE-VAKITPELKGSHGVMDPN
--NLELI-----E-E-----E--SMND-L-YK-VLARLSNGHAAI-IVR-EGS
117 AYNLI-IADYKDAEIEKLLADTVEYASMEPKLDYTPVKP--SN----ILI-RDEGP
-KM-RPLI---TENWYPIVRDITLA-L---S--E--T--L--PLE---K--ES--
175 FKEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGKVTESFH
-LKAYR---PDHGPYR--ED-DK-TLEP-----P-----T-VAFGR
233 TLCVFFLHKP-HKPGRDFERFDENTFTNSIQIARDPRFNFYFIADNDQITAVPRGD
-RWQK---VQED--GYK---EA-----T--E---A---KNL-----
291 ERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMSYY
-GQL-A--G--YHRENKWSKEVPLW-----A-Q---DLEDLVNWLTHIA-RK---
349 RGSLTAIEGVGY--E--KI-KEQ-LEKIYQPATQPGVDRGDLEFG--HIYVRKVG
---L-----V--S-----TY-----A--F---DFSYGEEKL-
407 KAALRLLAYLHHIHSVGGDSLLGFLHLSLGHQKVHNMALFTENRDFE-GERIAI
---LK-----GAACA---ESVGK--ESLDVDYWG---TF-----R--NEKN
465 NIRTL SQYVIRGAGINLHGVEESNGMQGEPLGVAE-GCAKLTTHPYENWYRDFNPKN
WQSE--GH---RV----LV-LKTVA---
523 AQAVANGYTEDRLAFGDLIILA-VPKKS

```

Matches with 33 **S62A** : 60 S \mapsto 35 S

3 Alignment of Schizosaccharomyces pombe's Mutations

align to reference sequence:

Compare sequences of length 108 and 211

```

NDILEKSVYKGDKDLHYVIPVGTALERKVIQDGTLGELDMILARLSNGHAAILVKE
1 -----
GKLIHPVITSKYYPVREATDKLSEGNPPAIDYSRRWIQVQEAGWKKRADDKNLQ
59 -----RR????????????????????
LDGYRENLKESKITELNPEGVEELIIQCTKQARQLASTFAIDFKYGRSKLREGGL
117 ?????RE????????????????????????????????????S????????????????????
KAEKIGTESLAPDKWGTFLNLKNWESEGHRTLVLNPAEETTM
175 ?????????????????????????????????????R-----

```

minimal editing distance: 30 Alignment: -1

3.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 211 and 511

```
V-ILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLLKIGKKTIVIVPVPNTTHATQPKG
1 NDILEKSVY-K---G--DK-----D-LHY-----VI-PVG-T--ALERKV
--DPTLVE-D---A---NGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKG
59 IQDGTLGELDMILARLSNGH-A--AI---L--V-K--EG-----K---LI-
SHGVMDPNAYNLIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGP
117 -HPV-----I-----T---S--KY-Y-P-----LVR-EA-
FEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAV-YGAVTESF
175 -----TD--K-----L-----S--EG--NP---P--AIDY-----SR
HTLCVFFLH-KPHKGR-DFERFDENTFTNSIQIARDPRFNFYFIADNDQITAVPR
233 RWIQVQVQAGWK--K--RAD----DKNLG---QL--DGY--Y-----R
GDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMS
291 --EN-----LK-ES---K---ITELN---P-EG-VE-----E-----
YYRGSLLTAIEGVGYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAAALRLL
349 -----L--I-----I--QCTK--Q-ARQ-----L-----ASTF--
AYLHHIHSVGGDSLLGFLHLSTGHQKVHMAALFTENRDFEGERIAINIRTLISQY
407 A---I-----DFKYGR--S---K-----L---R--EGG-----LK--
VIRGAG-INLHGVESNGMQEPLGVAEGCAKLTTHPYENWYRDF-NPKNAQAVANG
465 ----AEKI---GTES-----L--APD--KWGT-----FLNLKNWESE--G
YTEDR-LAFGDLIILAVPKKXX--
523 H---RTL---L--LN-PAAETTM
```

Matches with 32 **E93D** : 92 E → 241 E
R120Q : 119 R → 297 H
R120Q/R121Q : 119 R → 297 H
R121Q : 120 R → 298 F
R14Q : 13 R → 17 R
R94Q : 93 R → 244 R
S62A : 61 S → 136 A

3.2 Align To Sequence In 1e58.pdb

Compare sequences of length 211 and 248

```
KGQNAVAATAAKAI-EDANGLYRKLKPFNEDFEYVLPVGTPIINLEL--IEESMND
1 ---ND-----ILEKSV--Y--KGDK---DLHYVIPVGTGTA--LERKVIQDGTLGE
LYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESLKAY
59 LDMILARLSNGHAAIIVKEG-K---LIH----P-V--IT---S-----KY----Y
RPDHGYPYRED-DKTL-E--PPTVAFG--RRW-QKVQEDGYKE-ATEAKNLGQLAGY
117 -PLV---REATDK-LSEGNPP--AIDYSRRWIQ-VQEAGWKKRADD-KNLGQLDGY
HRENLKWSK--EVPLWAQDLEDLVNWLTHIARKLVSTYAFDFSYGEEKLLKGAAGA
175 YRENLKESKITE--LNPEGVVEELIIQCTKQARQLASTFAIDFKYGRSKLREGGLKA
ESVGKESLDVDYWGTFRNEKNWQSEGHRVVLVLTVA-----
233 EKIGTESLAPDKWGTFLNLKNWESEGHRVLLLNPAETTM
```

Matches with 51 **E93D** : 92 E \mapsto 88 E
R120Q : 119 R \mapsto 115 R
R120Q/R121Q : 119 R \mapsto 115 R
R121Q : 120 R \mapsto 116 R
R14Q : 13 R \mapsto 9 R
R94Q : 93 R \mapsto 89 R
S62A : 61 S \mapsto 57 S

4 Alignment of Schizosaccharomyces pombe's Mutations

align to reference sequence:

Compare sequences of length 1 and 211

```

1 NDILEKSVYKGDKDLHYVIPVGTALERKVIQDGTLGELDMILARLSNGHAAILVKE
-----
59 GKLIHPVITSKYYPVREATDKLSEGNPPAIDYSRRWIQVQEAGWKKRADDKNLGQ
-----
117 LDGYYrENLKESKITELNPEGVEELIIQCTKQARQLASTFAIDFKYGRSKLREGGL
-----
175 E-----
KAEKIGTESLAPDKWGTFLNLKNWESEGHRTLVLNPAAE'TM
-----

```

minimal editing distance: 30 Alignment: -1

4.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 211 and 511

```

1 V-ILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLLKIGKKTVIVPVPNTTHATQPKG
NDILEKSVY-K---G--DK-----D-LHY-----VI-PVG-T--ALERKV
--DPTLVE-D---A---NGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKG
59 IQDGTLGELDMILARLSNGH-A--AI---L---V-K--EG-----K---LI-
SHGVMDPNAYNLIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGP
117 -HPV-----I-----T---S---KY-Y-P-----LVR-EA-
FEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFVAV-YGAVTESF
175 -----TD---K-----L-----S--EG--NP---P--AIDY-----SR
HTLCVFFLH-KPHKGR-DFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPR
233 RWIQVQEAGWK--K--RAD---DKNLG---QL--DGY--Y-----R
GDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMS
291 --EN-----LK-ES---K---ITELN---P-EG-VE-----E-----
YYRGSLLTAIEGVGYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLL
349 ---L-I-----I--QCTK--Q-ARQ-----L-----ASTF--
AYLHHIHSVGGDSLLGFLHLSTGHQKVHMAALFTENRDFEGERIAINIRTLSQY
407 A---I-----DFKYGR--S---K-----L---R--EGG-----LK--
VIRGAG-INLHGVESNGMQGEPLGVAEGCAKLTTHPYENWYRDF-NPKNAQAVANG
465 ---AEKI---GTES-----L--APD--KWGT-----FLNLKNWESE--G

```

```

523 YTEDR-LAFGDLIILAVPKKXX--
      H---RTLVL---L--LN-PAAETTM

```

Matches with 32 **E93D** : 92 E \mapsto 241 E

4.2 Align To Sequence In 1e58.pdb

Compare sequences of length 211 and 248

```

1 KGQNAVAAAKAAI-EDANGLYRKLPKFNEDFEYVLPVGTPIINLEL--IEEESMND
  ---ND-----ILEKSV--Y--KGDK---DLHYVIPVGTAA--LERKVIQDGTLGE
  LYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESLKAY
59 LDMILARLSNGHAAIIVKEG-K---LIH-----P-V--IT---S-----KY----Y
  RPDHGPIYRED-DKTL-E--PPTVAFG--RRW-QKVQEDGYKE-ATEAKNLGQLAGY
117 -PLV---REATDK-LSEGNPP--AIDYSRRWIQ-VQEAGWKKRADD-KNLGQLDGY
  HRENLKWSK--EVPLWAQDLEDLVNWLTHIARKLVSTYAFDFSYGEEKLLKGAACA
175 YRENLKESKITE--LNPEGVEELIIQCTKQARQLASTFAIDFKYGRSKLREGGLKA
  ESGVKESLDVDYWGTFRNEKNWQSEGHRVVLVLTVA-----
233 EKIGTESLAPDKWGTFLNLKNWESEGHRTLVLNPAETTM

```

Matches with 51 **E93D** : 92 E \mapsto 88 E

5 Alignment of *Saccharomyces cerevisiae*'s Mutations

align to reference sequence:

Compare sequences of length 2 and 246

```

1 kKGQNAVAAAGAAAAEPDLYYSPKSPKLNEDLEFVLPIGTPIINLKAIDADSIGELH
  -----
  KVLGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPVYKYRE
59 -----LL-----
  DGKQSFPSADIPPPVDFSRRYTNFKEEGFKKLTAKDKGQLDGYHRENLRWSRN
  -----
117 VPIWLRDAKELAINATQIARSLKSTYLVDPYVKKEKLEGARAAEQQGKASLKVDV
  -----
175 WGTFLNKENWESQGHRVVLVKP
  -----
233 -----

```

minimal editing distance: 15 Alignment: -76

5.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 246 and 511

```

1 VILSKGTMEKQPGLGLL----DLMT-PA---L--DGLIGDRLKIGKKTIVVPVN
  K---KGQNAVAAA-GAAAAEPDLYYSPKSPKLNED-LEFV--LPIG--TPI----N

```

```

TTHATQPKGDPPTLVEDANGHDATIIAIGGKALIADVVKG-LCEDVAEVAKI--TPE
59 LK-AI----D-----A---DS-I---GE--LHK-VL-GRLSNGHA--A-IMVT--
LKSGSHGVMDPNAYNLIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRD
117 -KGS�-----L---D-K-A-IV---DQW-Y----P-L-----L-RD
EGPFEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDL-NTPKFAVYGAVT
175 I-----VL-----A--L-----S--E--TEPLVN-PD--VY----
ESFHTLCVFFLHKPHKPGRDFERFDENTFTNSIQIARDPRFNFYFIIADNDQITAVP
233 -----KY----R--E--DGKQ---SF-----PSS-----AD---IPP-P
RGDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDM
291 -----P-V--DF-----SR-----RYTNF-----KE-----
SYRGSLSLTAIEGVGYEKIKEQL-EKIYQPATQPGVDRGDLFGHIYVRKVGEKAALR
349 -----EGF---K-K--LTE-----AK----DKGQLDG--YHR---EN--LR
LLAYLHHIHSVGGDSLGLFLHLSTGHQKVNMAALFTENRDFEGERIAINIRTLS
407 W-----SRN-----VPIW--L----RDAK-EL-AINA-T--
QYVI-RGAGIN-LHGVESNGMQEPL--GV-A-E--GCAKLTTHPYENWYRDF-NP
465 Q--IARSLKSTYL--VDPYVKK-EKLLLEGARAAEQQKASLKVDV---WGT-FLN-
KNAQAVANGYTEDRLAFGLIILAVPKKXX-
523 KE-----NW--ESQ---GHRV-L-VLKP---

```

Matches with 32 **L245G** : 169 L \mapsto 397 L
L245G/L246G : 169 L \mapsto 397 L
L246G : 170 L \mapsto 407 H

5.2 Align To Sequence In 1e58.pdb

Compare sequences of length 246 and 248

```

K-GONAVAAAKAAI-E-DANGLYYR-KLPKFNEDEYVLPVGTIPINLELIEEESMN
1 KKGONAVAAAGAAAEPD---LYYSPKSPKLNEDLEFVLPIGTIPINLK AIDADSIG
DLYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESL-K
59 ELHKVLRGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPVYK
AYRPDHG----PYREDDKTLEPPTVAFGRRWQ--KVQEDGYKEATEAKNLGQLAGY
117 -YRED-GKQSFPSADIPP--PP-VDFSRRYTNFKE-E-GFKKLTEAKDKGQLDGY
HRENLKWSKEVPLWAQDL-EDLV-NWLTHIARKLVSTYAFDFSYGE-EKLLKGA-A
175 HRENLRWSRNVP IWL RDAKE-LAINA-TQIARSLKSTYLVDP-YVKK EKLLLEGARA
KAESVGKESLDVDYWGTFRNEK-NWQSEGHRVLVLKTVA-
233 -AEQQKASLKVDVWGTFLN-KENWESQGHRVLVLKP---

```

Matches with 59 **L245G** : 169 L \mapsto 172 M
L245G/L246G : 169 L \mapsto 172 M
L246G : 170 L \mapsto 173 K

6 Alignment of *Saccharomyces cerevisiae*'s Mutations

align to reference sequence:

Compare sequences of length 236 and 246

```

1 KKGQNAVAAGAAAAEPDLYSPKSPKLNEDLEFVLPVIGTPINLK AIDADSIGELH
K????????????????????????????????????????????????????????????
59 KVLGRLSNGHAAIMVTKGSLDKAIVDQWYPLLRDIVLALSETEPLVNPVYKYRE
????????????????????????????????????????????????????????????
117 DGKQSFPSADIPPPVDFSRRYTNFKEEGFKKLTEAKDKGQLDGYHRENLRWSRN
????????????????????????????????????????????????????????????
175 VPIWLRDAKELAINATQIARSLKSTYLVDVYVKKKLELEGARAAEQQGKASLKVDV
????????????????????????????????????????????????????????????
233 WGTFLNKENWeSQGHRVVLVLP
??????????????S-----

```

minimal editing distance: 0 Alignment: -1

6.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 246 and 511

```

1 VILSKGTMEKQPPLGLL----DLMT-PA---L--DGLIGDRLKIGKKTIVIVPVPN
K---KGQNAVAAA-GAAAAEPDLYSPKSPKLNED-LEFV--LPIG--TPI----N
TTHATQPKGDPTLVEDANGHDATIIAIGGKALIADVVKG-LCEDVAEVAKI--TPE
59 LK-AI----D-----A--DS-I--GE--LHK-VL-GRLSNGHA--A-IMVT--
LKGSHGVM DP NAYNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRD
117 -KGSL-----L--D-K-A-IV----DQW-Y----P-L-----L-RD
EGPFEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDL-NTPKFAVYGAVT
175 I-----VL-----A--L-----S--E--TEPLVN-PD--VY----
ESFHTLCVFFLHKPHKPGRDFERFDENTFTNSIQIARDPRFNFYFIADNDQITAVP
233 -----KY-----R--E--DGKQ--SF-----PSS-----AD---IPP-P
RGDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDM
291 -----P-V--DF-----SR-----RYTNF-----KE-----
SYRGSLSLTAIEGVGYEKIKEQL-EKIYQPATQPGVDRGDLFGHIYVRKVGEKAALR
349 -----EGF---K-K--LTE-----AK----DKGQLDG--YHR--EN--LR
LLAYLHHIHSVGGDSLLGFLHLSTGHQKVHNMALFTENRDFEGERIAINIRTLS
407 W-----SRN-----VPIW--L----RDAK-EL-AINA-T--
QYVI-RGAGIN-LHGVESNGMQGEPL--GV-A-E--GCAKLTTHPYENWYRDF-NP
465 Q--IARSLKSTYL--VDVYVKK-EKLELEGARAAEQQGKASLKVDV---WGT-FLN-
KNAQAVANGYTEDRLAFGDLIILAVPKKXX-
523 KE-----NW--ESQ---GHRV-L-VLKP---

```

Matches with 32 **K246G** : 245 K \mapsto 510 V
S11G : 10 S \mapsto 18 D

6.2 Align To Sequence In 1e58.pdb

Compare sequences of length 246 and 248

```

1 K-GQNAVAAAKAAI-E-DANGLYYR-KLPKFNEDEYVLPVIGTPINLELIEEESMN
KKGQNAVAAAGAAAAEPD---LYYSPKSPKLNEDLEFVLPVIGTPINLK AIDADSIG
DLYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESL-K

```

```

59 ELHKVLRGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPDVYK
AYRPDHG----PYREDDKTLEPPTVAFGRRWQ--KVQEDGYKEATEAKNLGQLAGY
117 -YRED-GKQSFSSADIPP--PP-VDFSRRYTNFKE-E-GFKKLTEAKDKGQLDGY
HRENLKWSKEVPLWAQDL-EDLV-NWLTHIARKLVSTYAFDFSYGE-EKLLKGA-A
175 HRENLRWSRNVP IWL RDAKE-LAINA-TQIARSLKSTYL VDP-YVKKEKLL EGARA
KAESVGKESLDVDYWGTFRNEK-NWQSEGHRVLVLKTVA-
233 -AEQQGKASLKVDVWGTFLN-KENWESQGHRVLVLKP---

```

Matches with 59 **K246G** : 245 K \mapsto 247 K
S11G : 10 S \mapsto 13 S

7 Alignment of *Saccharomyces cerevisiae*'s Mutations

align to reference sequence:

Compare sequences of length 76 and 246

```

KKGQNAVAAAAGAAAAEPDLYYSPKSPKLNEDLEFVLP IGTPI NLKAIDADSIGELH
1 -----
KVLGRGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPDVYKYRE
59 -----
DGKQSFSSADIPPPPVDDFSRRYTNFKEEGFKKLTEAKDKGQLDGYHRENLRWSRN
117 -----E????????
VPIWL RDAKELAINATQIARSLKSTYL VDPYVKKEKLL EGARAAEQQGKASLKVDV
175 ?????????????????A????????????????????????????????????
WGTFLNKENWESQGHRVLVLKP
233 ?????????????S-----

```

minimal editing distance: 30 Alignment: -1

7.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 246 and 511

```

VILSKGTMEKPQPLGLL----DLMT-PA---L--DGLIGGDRLKIGKKTIVIVPVPN
1 K---KGQNAVAAA-GAAAAEPDLYYSPKSPKLNED-LEFV--LPIG--TPI----N
TTHATQPKGDPTLVEDANGHDATIIAIGGKALIADVVKG-LCEDVAEVAKI--TPE
59 LK-AI----D-----A---DS-I---GE--LHK-VL-GRLSNGHA--A-IMVT--
LKSGSHGVMDPNAYNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRD
117 -KGS L-----L---D-K-A-IV----DQW-Y----P-L-----L-RD
EGPFEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDL-NTPKFAVYGAVT
175 I-----VL-----A--L-----S--E--TEPLVN-PD--VY----
ESFHTL CVFFLHKPHKPGRDFERFDENTFTNSIQIARDPRFNFYFIADNDQITAVP
233 -----KY-----R--E--DGKQ---SF-----PSS-----AD---IPP-P
RGDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDM
291 -----P-V--DF-----SR-----RYTNF-----KE-----
SYRGS LTAIEGVGYEKIKEQL-EKIYQPATQPGVDRGDLFGHIYVRKVG EKAALR
349 -----EGF---K-K--LTE-----AK-----DKGQLDG--YHR---EN--LR

```

```

LLAYLHHIHSVGGDSLLGFLHLSTGHQVHNMAALFTENRDFEGERIAINIRTL
407 W-----SRN-----VPIW--L----RDAK-EL-AINA-T--
QYVI-RGAGIN-LHGVE SNGMQGEPL--GV-A-E--GCAKLTTHPYENWYRDF-NP
465 Q--IARSLKSTYL--VDPYVKK-EKLEGGARAAEQQKASLKVDV---WGT-FLN-
KNAQAVANGYTEDRLAFGLIILAVPKKXX-
523 KE-----NW--ESQ---GHRV-L-VLKP---

```

Matches with 32 **A60S** : 59 A \mapsto 0 -
E86Q : 85 E \mapsto 139 E
S11A : 10 S \mapsto 18 D

7.2 Align To Sequence In 1e58.pdb

Compare sequences of length 246 and 248

```

K-GQNAVAAAKAAI-E-DANGLYYR-KLPKFNEFFEYVLPVGTPIINLELIEEESMN
1 KKQNAVAAAGAAAAEPD---LYYSPKSPKLNEDLEFVLPIGTPIINLK AIDADSIG
DLYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESL-K
59 ELHKVLGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPDVYK
AYRPDHG----PYREDDKTLEPPTVAFGRRWQ--KVQEDGYKEATEAKNLGQLAGY
117 -YRED-GKQSFSSADIPP--PP-VDFSRRYT NFKE-E-GFKKLTEAKDKGQLDGY
HRENKWSKEVPLWAQDL-EDLV-NWLTHIARKLVSTYAFDFSYGE-EKLLKGA-A
175 HRENLRWSRNVP IWL RDAKE-LAINA-TQIARSLKSTYLVDP-YVKK EKLEGGARA
KAESVGKESLDVDYWGTFRNEK-NWQSEGHRVLVLKTVA-
233 -AEQQGKASLKVDVWGTFLN-KENWESQGHRVLVLKP---

```

Matches with 59 **A60S** : 59 A \mapsto 62 A
E86Q : 85 E \mapsto 88 E
S11A : 10 S \mapsto 13 S

8 Alignment of Bacillus stearothermophilus's Mutations

align to reference sequence:

Compare sequences of length 451 and 510

```

KVILSKGTMEKQPQLGLLDLMT PALDGLIGDRLKIGKKTIVVPVNTTHATQPKG
1 -----H???????
DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
59 ??????????H?????????????????????????????????????????H?????????
YNLIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFKEERG GSM
117 ??????????????????????????????????????????????????????????????
FFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGKVTESFHTLCVFFLHK
175 ??????????????????????????????????????????????????????????????
PHKPGRDFERFDENTFTNSIQIARDPRFNFIADNDQITAVPRGDERVIVSPLVF
233 ??????????????????????????????R?????????????????????????????????
EDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDMSYYRGS LTAIEGV

```

```

291  ?????????????????????????????????????????????????????????????????????????????????
GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSHVGG
349  ?????????????????????????????????????????????????????????????????H??H?H??
DSLLGFLHLSTGHQKVNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGV
407  ?????????????????????????????????????????????????????????????????????H??
ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGLIIL
465  ?S????????????????????H????????????????????????????????????D----
AVPKKS
523  -----

```

minimal editing distance: 45 Alignment: -2

8.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 510 and 511

```

1  -VILSKGTMEKPQPLGLLDLMTPALDGLIGGDRLKIGKKTIVPVPNTTHATQPKG
DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
59  DPTLVEDANGHDATIIAIGGKALIADVVKGLCEDVAEVAKITPELKGSHGVMDPNA
YNLIIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFEEERGGSM
117  YNLIIADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRDEGPFKEERGGSM
FFTVPHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGAVTESFHTLCVFFLHK
175  FFTVPHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGKVTESFHTLCVFFLHK
PHKPGRDFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPRGDERVIVSPLVF
233  PHKPGRDFERFDENTFTNSIQIARDPRFNYFIIADNDQITAVPRGDERVIVSPLVF
EDYIGHKYSDEICELPDYTPGEGYVMARYAKEVRDWRKDRDMSYYRGSLSLAIEGV
291  EDYIGHKYSDEICELPDYTPGEGYVMARYAKEVRDWRKDRDMSYYRGSLSLAIEGV
GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSHVGG
349  GYEKIKEQLEKIYQPATQPGVDRGDLFGHIYVRKVGEKAALRLLAYLHHIHSHVGG
DSLLGFLHLSTGHQKVNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGV
407  DSLLGFLHLSTGHQKVNMAALFTENRDFEGERIAINIRTLSQYVIRGAGINLHGV
ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGLIIL
465  ESNGMQGEPLGVAEGCAKLTTHPYENWYRDFNPKNAQAVANGYTEDRLAFGLIIL
AVPKKXX-
523  AVPKKS--

```

- Matches with 99 D12N : 10 D ↔ 12 D
- H123N : 121 H ↔ 123 H
- H125N : 123 H ↔ 125 H
- H128N : 126 H ↔ 128 H
- H407N : 405 H ↔ 407 H
- H42N : 40 H ↔ 42 H
- H42N/H128N : 40 H ↔ 42 H
- H445N : 443 H ↔ 445 H
- H462N : 460 H ↔ 462 H
- H66N : 64 H ↔ 66 H
- R.261L : 259 R ↔ 261 R
- S62A : 60 S ↔ 62 S

8.2 Align To Sequence In 1e58.pdb

Compare sequences of length 510 and 248

```

1  K-----G-----QN-----A-----VAA-----A---KA
KVILSKGTMEKPPQLGLLDLMTPALDGLIGGDRLKIGKKTIVIVPVPNTTHATQPKG
AI---EDANGLYYR-----K-LP-----KFN-EDF-EYVL---PV--GT-----PI
59  DPTLVEDANGHDATIIAIGGKALIAADVVKGLCEDVAE-VAKITPELKGSHGVMDPN
--NLELI-----E-E-----E--SMND-L-YK-VLARLSNGHAAI-IVR-EGS
117  AYNLI-IADYKDAEIEKLLADTVEYASMEPKLDYTPVKP--SN----ILI-RDEGP
-KM-RPLI---TENWYPIVRDITLA-L---S--E--T--L--PLE----K--ES--
175  FKEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDLNTPKFAVYGVKVTESFH
-LKAYR---PDHGPYR--ED-DK-TLEP-----P-----T-VAFGR
233  TLCVFFLHKP-HKPGRDFERFDENTFTNSIQIARDPRFNFYFIADNDQITAVPRGD
-RWQK---VQED--GYK---EA-----T--E---A---KNL-----
291  ERVIVSPLVFEDYIGHKYSDEICELEPDRYTPGEGYVMARYAKEVDRWRKDRDMSYY
-GQL-A--G--YHRENLKWSKEVPLW-----A-Q---DLEDLVNWLTHIA-RK---
349  RGSLTAIEGVY--E--KI-KEQ-LEKIYQPATQPGVDRGDLFG---HIYVRKVGE
---L-----V--S-----TY-----A--F---DFSYGEEKL-
407  KAALRLLAYLHHIHSHVGGDSLLGFLHLSTGHQKVHNMAALFTENRDFE-GERIAI
----Lk-----GAAKA--ESVgK--ESLDVDYWG----TF-----R--NEKN
465  NIRTLSQYVIRGAGINLHGVESNGMQGEPLGVAE-GCAKLTTHPYENWYRDFNPKN
WQSE--GH---RV---LV-LKTVA---
523  AQAVANGYTEDRLAFGDLIILA-VPKKS

```

Matches with 33 D12N : 10 D \mapsto 0 -

```

H123N : 121 H  $\mapsto$  0 -
H125N : 123 H  $\mapsto$  0 -
H128N : 126 H  $\mapsto$  0 -
H407N : 405 H  $\mapsto$  0 -
H42N : 40 H  $\mapsto$  0 -
H42N/H128N : 40 H  $\mapsto$  0 -
H445N : 443 H  $\mapsto$  229 L
H462N : 460 H  $\mapsto$  0 -
H66N : 64 H  $\mapsto$  0 -
R261L : 259 R  $\mapsto$  0 -
S62A : 60 S  $\mapsto$  35 S

```

9 Alignment of Saccharomyces cerevisiae's Mutations

align to reference sequence:

Compare sequences of length 1 and 246

```

1  KKGQNAVAAAGAAAAEPDLYYSPKSPKLNEDLEFVLPIGTPIINLK AIDADSIGELH
-----
59  KVLGRLSNgHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPDVYKYRE
-----
H-----

```

```

117 DGKQSFSSADIPPPVDFSRRYTNFKEEGFKKLTEAKDKGQLDGYHRENLRWSRN
-----
VPIWLRDAKELAINATQIARSLKSTYLVDPYVKKEKLLLEGARAAEQQGKASLKVDV
175 -----
WGTFLNKENWESQGHRVVLVLP
233 -----

```

minimal editing distance: 30 Alignment: -1

9.1 Align To Sequence In 1ejj.pdb

Compare sequences of length 246 and 511

```

1 VILSKGTMEKPQPLGLL----DLMT-PA---L--DGLIGGDRLKIGKKTIVIVPVPN
K---KGQNAVAAA-GAAAAEPDLYYSPKSPKLNED-LEFV--LPIG--TPI----N
TTHATQPKGDPTLVEDANGHDATIIAIGGKALIADVVKG-LCEDVAEVAKI--TPE
59 LK-AI-----D-----A---DS-I---GE--LHK-VL-GRLSNGHA--A-IMVT--
LKGSHGVM DPNAYNLI IADYKDAEIEKLLADTVEYASMEPKLDYTPVKPSNILIRD
117 -KGS-----L---D-K-A-IV-----DQW-Y-----P-L-----L-RD
EGPFEEERGGSMFFTVHPYKETEAIRLQRLGHQSLVEGITNDL-NTPKFAVYGAVT
175 I-----VL-----A--L-----S--E--TEPLVN-PD--VY----
ESFHTLCVFFLHKPHKPGRDFERFDENTFTNSIQIARDPRFNFYIIADNDQITAVP
233 -----KY-----R--E--DGKQ---SF-----PSS-----AD---IPP-P
RGDERVIVSPLVFEDYIGHKYSDEICELPDRYTPGEGYVMARYAKEVRDWRKDRDM
291 -----P-V--DF-----SR-----RYTNF-----KE-----
SYYRGS LTAIEGVGYEKIKEQL-EKIYQPATQPGVDRGDLFGHIYVRKVGEKAALR
349 -----EGF---K-K--LTE-----AK----DKGQLDG--YHR--EN--LR
LLAYLHHIHSVGGDSSLGFLHLSTGHQKVHNMAALFTENRDFEGERIAINIRTLS
407 W-----SRN-----VPIW--L----RDAK-EL-AINA-T--
QYVI-RGAGIN-LHGVESNGMQGEPL--GV-A-E--GCAKLTTHPYENWYRDF-NP
465 Q--IARSLKSTYL--VDPYVKK-EKLLLEGARAAEQQGKASLKVDV---WGT-FLN-
KNAQAVANGYTEDRLAFGDLIILAVPKKXX-
523 KE-----NW--ESQ---GHRV-L-VLKP---

```

Matches with 32 H181A : 180 H → 421 V

9.2 Align To Sequence In 1e58.pdb

Compare sequences of length 246 and 248

```

1 K-GQNAVAAAKAAI-E-DANGLYYR-KLPKFNEDEYVLPVGTPIINLELIEEESMN
KKGQNAVAAA-GAAAAEPD---LYYSPKSPKLNEDLEFVLPVGTPIINLK AIDADSIG
59 DLYKVLARLSNGHAAIIVREGSKMRPLITENWYPIVRDITLALSETLPLEKESL-K
ELHKVLRGRLSNGHAAIMVTKGSLLDKAIVDQWYPLLRDIVLALSETEPLVNPDVYK
AYRPDHG----PYREDDKTLEPPTVAFGRRWQ--KVQEDGYKEATEAKNLGQLAGY
117 -YRED-GKQSFSSADIPP--PP-VDFSRRYTNFKE-E-GFKKLTEAKDKGQLDGY
HRENLKWSKEVPLWAQDL-EDLV-NWLTHIARKLVSTYAFDFSYGE-EKLLKGA-A
175 HRENLRWSRNVP IWL RDAKE-LAINA-TQIARSLKSTYLVDP-YVKKEKLLLEGARA

```

233 KAESVGKESLDVDYWGTFRNEK-NWQSEGHRVLVLKTVA-
-AEQQGKASLKVDVWGTFLN-KENWESQGHRVLVLKP---

Matches with 59 **H181A** : 180 H \mapsto 183 H