**Final\_\_\_:**

For Final\_\_ \_\_\_ (\_\_\_) was designed. The chains are always without the signal peptide and without the propeptide. First, the wild-type sequence of \_\_\_ is shown. The amino acids (aa) that are mutated are marked in red. In the line below the new aa are marked in green. The new sequence is at the end of the file. Here, the mutated aa are shown in green. The aa involved in binding to the target protein chymotrypsin are highlighted in yellow.

\_\_\_ tryptophan has been inserted into the mutant sequence out of a total of \_\_\_ mutations. The interaction score is \_\_\_ Rosetta Energy Units (REU). The total energy of the \_\_\_-Complex is -\_\_\_ REU. The surface area of the binding site of \_\_\_-Complex is \_\_\_ Å2 big. Other interesting values can be found in the Excel file.

M = AA to be mutated

M = inserted mutations

Interface environment

**Wild Type Fasta Sequence of \_\_\_**

**>sp|Q9FL28|24-1173**

|  |  |  |
| --- | --- | --- |
| 1 | KQSFEPEIEALKSFKNGISNDPLGVLSDWTIIGSLRHCNWTGITCDSTGHVVSVSLLEKQ | 60 |
| 61 | LEGVLSPAIANLTYLQVLDLTSNSFTGKIPAEIGKLTELNQLILYLNYFSGSIPSGIWEL | 120 |
| M | LEGVLSPAIANLTYLQVLDLTSNSFTGKIPAEIGKLTELNQLILALNYFSGSIPSGIWEL |  |
| 121 | KNIFYLDLRNNLLSGDVPEEICKTSSLVLIGFDYNNLTGKIPECLGDLVHLQMFVAAGNH | 180 |
| M | KNIFYLDLGNNLLSGDVPEEICKTSSLVLIVFDYNNLTGKIPECLGDLVHLELFVAAGNH |  |
| 181 | LTGSIPVSIGTLANLTDLDLSGNQLTGKIPRDFGNLLNLQSLVLTENLLEGDIPAEIGNC | 240 |
| M | LTGSIPVSIGTLANLKVLILSGNQLTGKIPRDFGNLLNLRILILTENLLEGDIPAEIGNC |  |
| 241 | SSLVQLELYDNQLTGKIPAELGNLVQLQALRIYKNKLTSSIPSSLFRLTQLTHLGLSENH | 300 |
| M | SSLQQLLLYDNQLTGKIPAELGNLVQLIILLIYKNKLTSSIPSSLFRLTQLLILVLAENH |  |
| 301 | LVGPISEEIGFLESLEVLTLHSNNFTGEFPQSITNLRNLTVLTVGFNNISGELPADLGLL | 360 |
| M | LVGPISEEIGFLESLRVLVLMSNNFTGEFPQSITNLRNLYILVVAFNNISGELPADLGLL |  |
| 361 | TNLRNLSAHDNLLTGPIPSSISNCTGLKLLDLSHNQMTGEIPRGFGRMNLTFISIGRNHF | 420 |
| M | TNLRILIAVFNLLTGPIPSSISNCTGLKILILAHNQMTGEIPRGFGRMNLTVIIIGRNHF |  |
| 421 | TGEIPDDIFNCSNLETLSVADNNLTGTLKPLIGKLQKLRILQVSYNSLTGPIPREIGNLK | 480 |
| M | TGEIPDDIFNCSNLEVLIVADNNLTGTLKPLIGKLQKLRILIVSYNSLTGPIPREIGNLK |  |
| 481 | DLNILYLHSNGFTGRIPREMSNLTLLQGLRMYSNDLEGPIPEEMFDMKLLSVLDLSNNKF | 540 |
| 541 | SGQIPALFSKLESLTYLSLQGNKFNGSIPASLKSLSLLNTFDISDNLLTGTIPGELLASL | 600 |
| 601 | KNMQLYLNFSNNLLTGTIPKELGKLEMVQEIDLSNNLFSGSIPRSLQACKNVFTLDFSQN | 660 |
| 661 | NLSGHIPDEVFQGMDMIISLNLSRNSFSGEIPQSFGNMTHLVSLDLSSNNLTGEIPESLA | 720 |
| 721 | NLSTLKHLKLASNNLKGHVPESGVFKNINASDLMGNTDLCGSKKPLKPCTIKQKSSHFSK | 780 |
| 781 | RTRVILIILGSAAALLLVLLLVLILTCCKKKEKKIENSSESSLPDLDSALKLKRFEPKEL | 840 |
| 841 | EQATDSFNSANIIGSSSLSTVYKGQLEDGTVIAVKVLNLKEFSAESDKWFYTEAKTLSQL | 900 |
| 901 | KHRNLVKILGFAWESGKTKALVLPFMENGNLEDTIHGSAAPIGSLLEKIDLCVHIASGID | 960 |
| 961 | YLHSGYGFPIVHCDLKPANILLDSDRVAHVSDFGTARILGFREDGSTTASTSAFEGTIGY | 1020 |
| 1021 | LAPEFAYMRKVTTKADVFSFGIIMMELMTKQRPTSLNDEDSQDMTLRQLVEKSIGNGRKG | 1080 |
| 1081 | MVRVLDMELGDSIVSLKQEEAIEDFLKLCLFCTSSRPEDRPDMNEILTHLMKLRGKANSF | 1140 |
| 1141 | REDRNEDREV | 1200 |

**>sp|Q94F62|26-615**

|  |  |  |
| --- | --- | --- |
| 1 | NAEGDALSALKNSLADPNKVLQSWDATLVTPCTWFHVTCNSDNSVTRVDLGNANLSGQLV | 60 |
| M | NAEGDALSALKNSLADPNKVLQSWDARLFLPCW |  |
| 61 | MQLGQLPNLQYLELYSNNITGTIPEQLGNLTELVSLDLYLNNLSGPIPSTLGRLKKLRFL | 120 |
| 121 | RLNNNSLSGEIPRSLTAVLTLQVLDLSNNPLTGDIPVNGSFSLFTPISFANTKLTPLPAS | 180 |
| 181 | PPPPISPTPPSPAGSNRITGAIAGGVAAGAALLFAVPAIALAWWRRKKPQDHFFDVPAEE | 240 |
| 241 | DPEVHLGQLKRFSLRELQVASDNFSNKNILGRGGFGKVYKGRLADGTLVAVKRLKEERTQ | 300 |
| 301 | GGELQFQTEVEMISMAVHRNLLRLRGFCMTPTERLLVYPYMANGSVASCLRERPESQPPL | 360 |
| 361 | DWPKRQRIALGSARGLAYLHDHCDPKIIHRDVKAANILLDEEFEAVVGDFGLAKLMDYKD | 420 |
| 421 | THVTTAVRGTIGHIAPEYLSTGKSSEKTDVFGYGVMLLELITGQRAFDLARLANDDDVML | 480 |
| 481 | LDWVKGLLKEKKLEALVDVDLQGNYKDEEVEQLIQVALLCTQSSPMERPKMSEVVRMLEG | 540 |
| 541 | DGLAERWEEWQKEEMFRQDFNYPTHHPAVSGWIIGDSTSQIENEYPSGPR | 600 |

**Inserted Peptide**

>Peptide 6ZOZ, 762-782

QLNRALTGIAVEQDKNTQEVF

**Mutations**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Positions chain A (FLS2)** | **From** | **To** | **Positions chain A (FLS2)** | **From** | **To** | **Positions chain A (FLS2)** | **From** | **To** |
|  |  |  |  |  |  |  |  |  |
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| --- | --- | --- |
| **Poisitions Chain B (BAK1)** | **From** | **To** |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

**Mutant Fasta Sequence**

**>Final\_\_\_\_, Chain\_A FLS2**

|  |  |  |
| --- | --- | --- |
| 1 | KQSFEPEIEALKSFKNGISNDPLGVLSDWTIIGSLRHCNWTGITCDSTGHVVSVSLLEKQ | 60 |
| 61 | LEGVLSPAIANLTYLQVLDLTSNSFTGKIPAEIGKLTELNQLILALNYFSGSIPSGIWEL | 120 |
| 121 | KNIFYLDLGNNLLSGDVPEEICKTSSLVLIVFDYNNLTGKIPECLGDLVHLELFVAAGNH | 180 |
| 181 | LTGSIPVSIGTLANLKVLILSGNQLTGKIPRDFGNLLNLRILILTENLLEGDIPAEIGNC | 240 |
| 241 | SSLQQLLLYDNQLTGKIPAELGNLVQLIILLIYKNKLTSSIPSSLFRLTQLLILVLAENH | 300 |
| 301 | LVGPISEEIGFLESLRVLVLMSNNFTGEFPQSITNLRNLYILVVAFNNISGELPADLGLL | 360 |
| 361 | TNLRILIAVFNLLTGPIPSSISNCTGLKILILAHNQMTGEIPRGFGRMNLTVIIIGRNHF | 420 |
| 421 | TGEIPDDIFNCSNLEVLIVADNNLTGTLKPLIGKLQKLRILIVSYNSLTGPIPREIGNLK | 480 |
| 481 | DLNILYLHSNGFTGRIPREMSNLTLLQGLRMYSNDLEGPIPEEMFDMKLLSVLDLSNNKF | 540 |
| 541 | SGQIPALFSKLESLTYLSLQGNKFNGSIPASLKSLSLLNTFDISDNLLTGTIPGELLASL | 600 |
| 601 | KNMQLYLNFSNNLLTGTIPKELGKLEMVQEIDLSNNLFSGSIPRSLQACKNVFTLDFSQN | 660 |
| 661 | NLSGHIPDEVFQGMDMIISLNLSRNSFSGEIPQSFGNMTHLVSLDLSSNNLTGEIPESLA | 720 |
| 721 | NLSTLKHLKLASNNLKGHVPESGVFKNINASDLMGNTDLCGSKKPLKPCTIKQKSSHFSK | 780 |
| 781 | RTRVILIILGSAAALLLVLLLVLILTCCKKKEKKIENSSESSLPDLDSALKLKRFEPKEL | 840 |
| 841 | EQATDSFNSANIIGSSSLSTVYKGQLEDGTVIAVKVLNLKEFSAESDKWFYTEAKTLSQL | 900 |
| 901 | KHRNLVKILGFAWESGKTKALVLPFMENGNLEDTIHGSAAPIGSLLEKIDLCVHIASGID | 960 |
| 961 | YLHSGYGFPIVHCDLKPANILLDSDRVAHVSDFGTARILGFREDGSTTASTSAFEGTIGY | 1020 |
| 1021 | LAPEFAYMRKVTTKADVFSFGIIMMELMTKQRPTSLNDEDSQDMTLRQLVEKSIGNGRKG | 1080 |
| 1081 | MVRVLDMELGDSIVSLKQEEAIEDFLKLCLFCTSSRPEDRPDMNEILTHLMKLRGKANSF | 1140 |
| 1141 | REDRNEDREV | 1200 |

**>Final\_\_\_\_, Chain B (BAK1)**

|  |  |  |
| --- | --- | --- |
| 1 | NAEGDALSALKNSLADPNKVLQSWDARLFLPCWWFHVTCNSDNSVTRVDLGNANLSGQLV | 60 |
| 61 | MQLGQLPNLQYLELYSNNITGTIPEQLGNLTELVSLDLYLNNLSGPIPSTLGRLKKLRFL | 120 |
| 121 | RLNNNSLSGEIPRSLTAVLTLQVLDLSNNPLTGDIPVNGSFSLFTPISFANTKLTPLPAS | 180 |
| 181 | PPPPISPTPPSPAGSNRITGAIAGGVAAGAALLFAVPAIALAWWRRKKPQDHFFDVPAEE | 240 |
| 241 | DPEVHLGQLKRFSLRELQVASDNFSNKNILGRGGFGKVYKGRLADGTLVAVKRLKEERTQ | 300 |
| 301 | GGELQFQTEVEMISMAVHRNLLRLRGFCMTPTERLLVYPYMANGSVASCLRERPESQPPL | 360 |
| 361 | DWPKRQRIALGSARGLAYLHDHCDPKIIHRDVKAANILLDEEFEAVVGDFGLAKLMDYKD | 420 |
| 421 | THVTTAVRGTIGHIAPEYLSTGKSSEKTDVFGYGVMLLELITGQRAFDLARLANDDDVML | 480 |
| 481 | LDWVKGLLKEKKLEALVDVDLQGNYKDEEVEQLIQVALLCTQSSPMERPKMSEVVRMLEG | 540 |
| 541 | DGLAERWEEWQKEEMFRQDFNYPTHHPAVSGWIIGDSTSQIENEYPSGPR | 600 |