Table : Percentage Sequence Identity Matrix (PSIM)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Xa1** | **Xa4** | **Xa5** | **Xa10** | **Xa13** | **Xa15** | **Xa19** | **Xa20** | **Xa21** | **Xa23** | **Xa25** | **Xa26** | **Xa27** |
| **Xa1** | 100 | - | - | - | - | 31.17 | 31.17 | 31.17 | 32.47 | - | 50.00 | 23.85 | 45.45 |
| **Xa4** | - | 100 | - | - | - | 28.00 | 26.09 | 28.00 | 24.11 | - | - | 27.56 | - |
| **Xa5** | - | - | 100 | - | - | 62.50 | 62.50 | 62.50 | 20.45 | - | - | - | - |
| **Xa10** | - | - | - | 100 | - | - | - | - | - | 35.78 | - | - | - |
| **Xa13** | - | - | - | - | 100 | - | - | - | - | - | 56.48 | 53.85 | 27.69 |
| **Xa15** | 27.74 | 60.87 | 62.50 | - | - | 100 | 99.17 | 99.72 | 98.07 | - | - | 36.76 | - |
| **Xa19** | 27.74 | 60.87 | 62.50 | - | - | 99.17 | 100 | 98.90 | 98.35 | - | 33.33 | 36.76 | - |
| **Xa20** | 27.74 | 60.87 | 62.50 | - | - | 99.72 | 98.90 | 100 | 97.80 | - | - | 36.49 | - |
| **Xa21** | 28.68 | 28.15 | 62.50 | - | - | 98.07 | 98.35 | 97.80 | 100 | - | 35.48 | 34.85 | - |
| **Xa23** | - | - | - | 35.78 | - | - | - | - | - | 100 | - | - | - |
| **Xa25** | 50.00 | - | - | - | 56.48 | - | 33.33 | - | 35.48 | - | 100 | - | - |
| **Xa26** | 23.49 | 27.56 | - | - | 53.85 | 36.76 | 36.76 | 36.49 | 37.22 | - | - | 100 | 27.59 |
| **Xa27** | 45.45 | - | - | - | 27.69 | - | - | - | - | - | - | 66.67 | 100 |

Table : Selected templates for homology modeling from BLAST against PDB database

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sr. No.** | **Templates** | **Total score** | **Identity (%)** | **Query coverage (%)** | **E value** | **Resolution (Ao)** |
| 1 | 4mn8\_A (for Xa15) | 1013 | 36.54 | 69 | 7e-21 | 3.06 |
| 2 | 6s6q\_A | 1414 | 40.96 | 73 | 1e-40 | 2.95 |
| 3 | 5hyx\_B | 696 | 38.13 | 84 | 1e-39 | 2.60 |
| 4 | 5gr8\_A | 1233 | 38.55 | 98 | 6e-36 | 2.59 |
| 5 | 4mn8\_A (for Xa19) | 1007 | 36.54 | 69 | 1e-40 | 3.06 |
| 6 | 6s6q\_A | 1408 | 40.96 | 73 | 2e-40 | 2.95 |
| 7 | 5hyx\_B | 819 | 38.13 | 84 | 2e-39 | 2.60 |
| 8 | 5gr8\_A | 1226 | 38.55 | 98 | 9e-36 | 2.59 |
| 9 | 4mn8\_A (for Xa20) | 1123 | 36.21 | 69 | 1e-40 | 3.06 |
| 10 | 6s6q\_A | 1326 | 40.56 | 73 | 2e-40 | 2.95 |
| 11 | 5hyx\_B | 694 | 38.13 | 84 | 2e-39 | 2.60 |
| 12 | 5gr8\_A | 1353 | 38.55 | 98 | 7e-36 | 2.59 |
| 13 | 4mn8\_A (for Xa21) | 917 | 32.69 | 58 | 6e-92 | 3.06 |
| 14 | 6s6q\_A | 1073 | 36.79 | 66 | 6e-84 | 2.95 |
| 15 | 5hyx\_B | 267 | 33.86 | 56 | 2e-77 | 2.60 |
| 16 | 5gr8\_A | 463 | 32.28 | 57 | 7e-73 | 2.59 |

Table : Secondary structure comparison of selected templates and predicted models

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sr. No.** | **Target/ template** | **Number of amino acid residues (%)** | | | | **Total No. of amino acids** |
| **Turn** | **Helix** | **Strand** | **Coils** |
| 1 | Xa15 | 4.13 | 34.44 | 14.88 | 46.56 | 363 |
| 2 | Xa19 | 4.41 | 34.71 | 13.22 | 47.66 | 363 |
| 3 | Xa20 | 4.68 | 32.51 | 16.25 | 46.56 | 363 |
| 4 | Xa21 | 4.29 | 35.32 | 14.54 | 45.85 | 1025 |
| 5 | 6s6q | 1.39 | 38.24 | 9.50 | 50.87 | 863 |
| 6 | 4mn8 | 1.28 | 40.54 | 10.36 | 47.83 | 782 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sr. #** | **Protein Name** | **Model length (No. of Residues)** | **Amino-acid Residues in** | | | |
| **Most Favored regions** | **Additional Allowed regions** | **Generously Allowed regions** | **Disallowed regions** |
| **1.** | Xa15 | 262 | 75.0% | 53 | 2 | 0 |
| **2.** | Xa19 | 262 | 75.0% | 53 | 2 | 0 |
| **3.** | Xa20 | 262 | 75.0% | 53 | 2 | 0 |
| **4.** | Xa21 | 602 | 80.9% | 92 | 5 | 2 |
| **5.** | 6s6q.2 | 857 | 74.2% | 189 | 4 | 1 |
| **6.** | 4mn8.1 | 971 | 82.8% | 134 | 6 | 3 |

Table : Ramachandran plot result elucidation