**Table S1.** Comparison of types and number of interactions between E6, its variants and our models of MAGI-1. Hydrogen bonds, Salt bridges, Non-bonded contacts.

|  |  |  |  |
| --- | --- | --- | --- |
| **Complexes** | **Hydrogen bonds** | **Salt bridges** | **Non-bonded contacts** |
| **E6R/MAGI-1 255** | **9** | **3** | **156** |
| **E-G350/MAGI-1 255** | **14** | **9** | **156** |
| **E-C188/G350 /MAGI-1 255** | **25** | **7** | **231** |
| **E-A176/G350/ MAGI-1 255** | **23** | **10** | **382** |
| **AAa/MAGI-1 255** | **17** | **3** | **239** |
| **AAc/MAGI-1 255** | **13** | **2** | **199** |
| **Complexes** | **Hydrogen bonds** | **Salt bridges** | **Non-bonded contacts** |
| **E6R/MAGI-1 329** | **11** | **6** | **156** |
| **E-G350/MAGI-1 329** | **18** | **4** | **220** |
| **E-C188/G350 /MAGI-1 329** | **23** | **8** | **298** |
| **E-A176/G350/ MAGI-1 329** | **18** | **5** | **212** |
| **AAa/MAGI-1 329** | **24** | **8** | **242** |
| **AAc/MAGI-1 329** | **12** | **6** | **189** |

**Table S2.** Detailed results of amino acidic interaction between E6, its variants and our two MAGI-1 models.

|  |  |  |
| --- | --- | --- |
| **E6 VPH-16** | **Residues** | **Residues MAGI1-1 255** |
| **E6-referece** | **Y81, R10, C30, R77, V31, Y32, R55, Y76, C66, A61, F69, K65, V62, V53, L67, N127, C51, C80, R131, G130, Q107, I73, R129 and Y70.** | **G75, A234, Y74, T161, N163, V79, D80, W66, G65, A64, Y78, I76, H231, G230, Y77, E61, G70, K68 and E67.** |
| **E-G350** | **L72, R146, K68, N105, S143, E75, R135, S142, C139, S138, R144, C106, D44, E114, E113, M137, K121, R117, R141 and C140.** | **D57, S58, E59, L60, E61, P63, E55, L56, L62, A64, G65, Y78, K68, W66, D80, V79, E67 and H81.** |
| **E-C188/G350** | **R146, T145, K72, R144, R141, E150, S82, R147, E75, R124, R135, Y84, E148, Y79, H78, R77, Y76, F69, C82, R129, Y70, Y81, G130, N127,Y92 and R131.** | **S58, D57, L62, E67, L60, E59, P63, R162, A64, E61, L56, E54, E55, L167, S165, P164, N163, F160, K230, P193, F196, L229, D194, E70, K68, V221, N224, Q235, S222, C227, F171 and D225.** |
| **E-A176/G350** | **R146, Y84, N105, R124, R147, E148, S82, Y81, Q90, Q91, C33, T145, S143, R131, R129, S142, C80, G130, R77, I73, Y79, Y76, E75, K72, S74, S71, K68, D64, P69, K34, L67, K65, C66, C63, Y70, V62, R55, D56, Y32 and V53.** | **E55, A64, L167, N163, E54, P164, S165, R162, C227, D225, K85, T226, L229, L60, E61, P63, E70, E59, H231, P193, G230, D194, F159, F196, K68, F160, E67, V79, I69, Y78, H81, D80, R84, Y77, E151, N83, Y88, Y74, I82, E89, Q87, T86, E94, N90, P91 and R150.** |
| **AAa** | **R131, R29, S143, R10, Y32, Y70, F69, S74, R55, I73, Y76, Y78, R77, G130, Y92, K72, W132, N127, Y81, L151, E148, E75, Y79, R144, R124, S82, R147 and H126.** | **E67, W66, K238, E166, L62, P164, R162, L167, N163, F171, E59, S165, D194, T161, F196, F160, E195, I82, F159, K157, K68, C227, E70, I243, L229, P244, Q241, Q122, S242, G230, H231 and Q119.** |
| **AAc** | **C80, R129, R135, H126, Y81, G130, Y79, Y78,Y76, R124, E75, S82, R77, Y84, V83, Y32, Y70, F69, Q91, K72 and K65.** | **V221, C227, N163, H231, F171, E252, L229, T161, P164, G230, R162, S165, F160, F196, D194, F159, I76, I82, L167, E70, K168, K68 and E67.** |
|  | **Residues** | **Residues MAGI-1 329** |
| **E6-referece** | **D64, K72, K68, K65, Y76, R147, F69, I73, L50, R77, Y70, R129, H78, V62, Q17, L67, R131, C66, V31, D56, Y32, R55 and V53.** | **D57, E54, S58, K157, A64, L62, E65, T53, G65, W66, V79, Y78, H81, I82, E67, D80, V92, E94, N83, R97, P91, N90 and E89.** |
| **E-G350** | **R77, I73, R129, Y76, D56, H78, I128, Y70, S71, N105, R48, C66, L67, I104, Q107, D74, L50, R131, Y32, F69, K72, R55, V31, V53 and K34.** | **A64, W66,G65, Q106, Y78, I69, K68, E61, E67, V79, T86, R84, H81, I82, D80, L93, E94, V92, T53, E54, D57, E102, R97, Q105, L101 and Q110.** |
| **E-C188/G350** | **K72, E75, R77, Y76, S142, R144, M137, R117, S143, R141, C140, K68, K65, F69, D64, E148, R147, T145, T149, R146, L151 and Q150.** | **S269, L270, V284, N285, G286, E55, E59, V51, Q39, F261, D262, L60, V317, D316, T272, T26, N23, T24, R33, E280, P263, N36, D265, P41, H22, D264, L35, L42, N145, D21, E43, E151, T12, L25, Y11, A10, E13, E8, M9 and I20.** |
| **E-A176/G350** | **R147, Y32, R55, G57, Y70, I73, K72, F69, S71, S74, Q91, E75, I128, Y79, H126, Y76, H78, R77, V83, R129, R131, C80, S82, R124 and Y81.** | **E89, L62, Q87, D316, E61, K157, A64, Y78, T86, W66, G65, V79, E67, D80, D57, Q106, H81, N83, I82, R84, P91, T53, H52, E94, N90, E54, L93, V92, and R97.** |
| **AAa** | **R77, Y76, K72, E75, Y79, R135, S138, S143, R141, S142, L151, K121, R144, T145, Q150, R147, E148, T149 and R146.** | **L277, E321, D278, V317, A318, D316, A315, N320, L6, L154, S58, E61, E59, L60, P260, K200, L259, P153, V51, V188, D262, F261, D264, L35, P263, Q39, K40, C34, P41, L42, E43, H52, G50 and E55.** |
| **AAc** | **K65, K68, F69, Y78, R129, S74, R77, L50, V62, Y70, I73, R102, Q107, F45, L67, V53, Y32, Y76, Y60, K72, D56, C33, V31, K34 and R55.** | **T53, E54, S58, D57, L56, Y78, D80, I69, K68, E67, V79, H81, I82, E94, W66, A64, G65, N83, L62, R84, R97, K157, E61, L93, V92, L101, N90 and E89.** |