**Ternary (Open vs Closed)**

Residues with significant energy change between conformations

|  |  |  |  |
| --- | --- | --- | --- |
| **RESID** | **Open** | **Closed** | **Delta** |
| ALA\_146 | -39.77 | -35.64 | -4.13 |
| ASN\_229 | -82.86 | -76.42 | -6.44 |
| ASP\_346 | -69.21 | -67.04 | -2.17 |
| GLN\_169 | -81.17 | -70.16 | -11.01 |
| GLN\_170 | -76.16 | -68.09 | -8.07 |
| GLU\_198 | -64.7 | -54.49 | -10.21 |
| GLU\_323 | -55.36 | -52.36 | -3 |
| GLY\_319 | -45.48 | -42.77 | -2.71 |
| ILE\_154 | -21.93 | -16.94 | -4.99 |
| ILE\_230 | -29.75 | -27.02 | -2.73 |
| ILE\_291 | -36.38 | -34.28 | -2.1 |
| LEU\_168 | -47.52 | -43.67 | -3.85 |
| LEU\_182 | -19.42 | -17.16 | -2.26 |
| PHE\_180 | -47.35 | -45.13 | -2.22 |
| PHE\_294 | -41.29 | -38.2 | -3.09 |
| PRO\_155 | -21.21 | -11.97 | -9.24 |
| PRO\_160 | -11.17 | -7.81 | -3.36 |
| PRO\_191 | -21.6 | -19.41 | -2.19 |
| SER\_149 | -45.93 | -42.94 | -2.99 |
| SER\_166 | -34.42 | -32.18 | -2.24 |
| THR\_194 | -41.84 | -37.51 | -4.33 |
| THR\_227 | -47.14 | -44.16 | -2.98 |
| TYR\_171 | -43.84 | -39.14 | -4.7 |
| VAL\_292 | -38.37 | -35.24 | -3.13 |

Physical interpretation of change in energy

*Here, MC represents main chain contact, SC represents Side chain contacts, and PIPISTACK signifies π-π stacking interactions between a pair of residues I & J*

|  |  |  |
| --- | --- | --- |
| **RESIDUE (I) open** | **Interaction** | **RESIDUE (J) open** |
| **A:146:\_:ALA** | **HBOND:MC\_MC** | **A:149:\_:SER** |
| **A:146:\_:ALA** | **HBOND:MC\_MC** | **A:150:\_:THR** |
| **A:146:\_:ALA** | **VDW:SC\_SC** | **A:156:\_:ASP** |
| **A:154:\_:ILE** | **VDW:SC\_SC** | **A:199:\_:LEU** |
| **A:154:\_:ILE** | **VDW:SC\_SC** | **A:204:\_:TYR** |
| **A:154:\_:ILE** | **VDW:SC\_SC** | **A:231:\_:ASP** |
| **A:154:\_:ILE** | **VDW:SC\_SC** | **A:233:\_:LEU** |
| **A:155:\_:PRO** | **VDW:SC\_SC** | **A:160:\_:PRO** |
| **A:155:\_:PRO** | **VDW:SC\_SC** | **A:164:\_:LEU** |
| **A:158:\_:ARG** | **VDW:SC\_SC** | **A:165:\_:TYR** |
| **A:158:\_:ARG** | **VDW:SC\_SC** | **A:168:\_:LEU** |
| **A:158:\_:ARG** | **VDW:SC\_SC** | **A:176:\_:PRO** |
| **A:171:\_:TYR** | **VDW:SC\_SC** | **A:190:\_:LYS** |
| **A:171:\_:TYR** | **VDW:SC\_SC** | **A:191:\_:PRO** |
| **A:175:\_:TYR** | **HBOND:MC\_MC** | **A:178:\_:ALA** |
| **A:175:\_:TYR** | **VDW:SC\_SC** | **A:178:\_:ALA** |
| **A:175:\_:TYR** | **HBOND:SC\_SC** | **A:181:\_:GLU** |
| **A:177:\_:GLU** | **HBOND:MC\_MC** | **A:180:\_:PHE** |
| **A:177:\_:GLU** | **VDW:SC\_SC** | **A:294:\_:PHE** |
| **A:194:\_:THR** | **HBOND:MC\_MC** | **A:198:\_:GLU** |
| **A:198:\_:GLU** | **HBOND:MC\_SC** | **A:203:\_:ASN** |
| **A:198:\_:GLU** | **VDW:MC\_SC** | **A:203:\_:ASN** |
| **A:198:\_:GLU** | **VDW:MC\_SC** | **A:204:\_:TYR** |
| **A:210:\_:HIS** | **HBOND:MC\_MC** | **A:213:\_:LEU** |
| **A:210:\_:HIS** | **HBOND:MC\_MC** | **A:214:\_:ARG** |
| **A:210:\_:HIS** | **VDW:SC\_SC** | **A:233:\_:LEU** |
| **A:210:\_:HIS** | **VDW:SC\_SC** | **A:237:\_:SER** |
| **A:228:\_:GLN** | **VDW:SC\_SC** | **A:248:\_:HIS** |
| **A:228:\_:GLN** | **HBOND:SC\_SC** | **A:320:\_:THR** |
| **A:228:\_:GLN** | **VDW:SC\_SC** | **A:324:\_:VAL** |
| **A:228:\_:GLN** | **VDW:SC\_SC** | **A:327:\_:PHE** |
| **A:234:\_:GLU** | **HBOND:MC\_SC** | **A:237:\_:SER** |
| **A:234:\_:GLU** | **HBOND:MC\_MC** | **A:239:\_:ILE** |
| **A:234:\_:GLU** | **VDW:SC\_SC** | **A:244:\_:LEU** |
| **A:320:\_:THR** | **HBOND:MC\_SC** | **A:344:\_:ASN** |

|  |  |  |
| --- | --- | --- |
| **RESIDUE (I)Closed** | **Interaction** | **RESIDUE (J) Closed** |
| A:146:\_:ALA | HBOND:MC\_MC | A:149:\_:SER |
| A:146:\_:ALA | HBOND:MC\_MC | A:150:\_:THR |
| A:146:\_:ALA | VDW:MC\_SC | A:156:\_:ASP |
| A:146:\_:ALA | VDW:SC\_SC | A:157:\_:PHE |
| A:146:\_:ALA | VDW:SC\_SC | A:229:\_:ASN |
| A:154:\_:ILE | VDW:SC\_SC | A:199:\_:LEU |
| A:154:\_:ILE | VDW:SC\_SC | A:204:\_:TYR |
| A:154:\_:ILE | VDW:SC\_SC | A:231:\_:ASP |
| A:154:\_:ILE | VDW:SC\_SC | A:233:\_:LEU |
| A:155:\_:PRO | VDW:SC\_MC | A:163:\_:GLY |
| A:156:\_:ASP | HBOND:SC\_MC | A:159:\_:SER |
| A:156:\_:ASP | VDW:SC\_SC | A:159:\_:SER |
| A:156:\_:ASP | HBOND:MC\_MC | A:162:\_:SER |
| A:156:\_:ASP | VDW:SC\_MC | A:162:\_:SER |
| A:156:\_:ASP | HBOND:MC\_MC | A:164:\_:LEU |
| A:157:\_:PHE | VDW:MC\_MC | A:163:\_:GLY |
| A:157:\_:PHE | VDW:SC\_SC | A:164:\_:LEU |
| A:157:\_:PHE | HBOND:MC\_MC | A:165:\_:TYR |
| A:157:\_:PHE | PIPISTACK:SC\_SC | A:165:\_:TYR |
| A:157:\_:PHE | VDW:SC\_SC | A:165:\_:TYR |
| A:157:\_:PHE | PIPISTACK:SC\_SC | A:180:\_:PHE |
| A:157:\_:PHE | VDW:SC\_SC | A:180:\_:PHE |
| A:158:\_:ARG | VDW:SC\_SC | A:165:\_:TYR |
| A:158:\_:ARG | IONIC:SC\_SC | A:177:\_:GLU |
| A:158:\_:ARG | HBOND:SC\_SC | A:177:\_:GLU |
| A:158:\_:ARG | HBOND:SC\_SC | A:323:\_:GLU |
| A:159:\_:SER | HBOND:MC\_MC | A:163:\_:GLY |
| A:159:\_:SER | HBOND:SC\_SC | A:345:\_:ARG |
| A:163:\_:GLY | HBOND:MC\_SC | A:166:\_:SER |
| A:163:\_:GLY | HBOND:MC\_SC | A:167:\_:ASN |
| A:163:\_:GLY | VDW:MC\_SC | A:167:\_:ASN |
| A:169:\_:GLN | VDW:SC\_SC | A:176:\_:PRO |
| A:171:\_:TYR | VDW:SC\_SC | A:179:\_:ILE |
| A:171:\_:TYR | VDW:SC\_SC | A:191:\_:PRO |
| A:171:\_:TYR | VDW:SC\_SC | A:194:\_:THR |
| A:171:\_:TYR | HBOND:SC\_SC | A:198:\_:GLU |
| A:175:\_:TYR | HBOND:MC\_MC | A:178:\_:ALA |
| A:175:\_:TYR | VDW:SC\_SC | A:178:\_:ALA |
| A:175:\_:TYR | HBOND:SC\_SC | A:181:\_:GLU |
| A:177:\_:GLU | HBOND:MC\_MC | A:180:\_:PHE |
| A:177:\_:GLU | VDW:SC\_SC | A:294:\_:PHE |
| A:194:\_:THR | HBOND:MC\_MC | A:197:\_:LYS |
| A:194:\_:THR | VDW:MC\_SC | A:197:\_:LYS |
| A:194:\_:THR | HBOND:MC\_MC | A:198:\_:GLU |
| A:198:\_:GLU | HBOND:MC\_SC | A:203:\_:ASN |
| A:198:\_:GLU | VDW:MC\_SC | A:204:\_:TYR |
| A:210:\_:HIS | HBOND:MC\_MC | A:213:\_:LEU |
| A:210:\_:HIS | HBOND:MC\_MC | A:214:\_:ARG |
| A:210:\_:HIS | VDW:SC\_SC | A:233:\_:LEU |
| A:210:\_:HIS | VDW:SC\_SC | A:237:\_:SER |
| A:228:\_:GLN | HBOND:MC\_SC | A:248:\_:HIS |
| A:228:\_:GLN | VDW:SC\_SC | A:248:\_:HIS |
| A:228:\_:GLN | HBOND:SC\_SC | A:320:\_:THR |
| A:228:\_:GLN | VDW:SC\_SC | A:324:\_:VAL |
| A:228:\_:GLN | VDW:SC\_SC | A:327:\_:PHE |
| A:229:\_:ASN | HBOND:SC\_SC | A:234:\_:GLU |
| A:229:\_:ASN | VDW:SC\_SC | A:234:\_:GLU |
| A:234:\_:GLU | HBOND:MC\_SC | A:237:\_:SER |
| A:234:\_:GLU | VDW:SC\_SC | A:244:\_:LEU |
| A:320:\_:THR | HBOND:MC\_SC | A:344:\_:ASN |

***NB: I will modify this list by removing the common interaction in open and closed***

**Sirt3/INT Complex**

Residues with significant energy change between conformations

|  |  |  |  |
| --- | --- | --- | --- |
| **RESID (4BVG open vs closed** | **Native(closed)** | **Model(open)** | **Delta** |
| A:GLY\_163 | -38.28 | -29.01 | -9.27 |
| A:PHE\_157 | -39.19 | -32.34 | -6.85 |
| A:LEU\_199 | -36.99 | -41.59 | 4.6 |
| A:PRO\_160 | -7.46 | -12.5 | 5.04 |
| A:THR\_194 | -36.41 | -41.47 | 5.06 |
| A:TYR\_171 | -39.36 | -44.64 | 5.28 |
| A:ASP\_172 | -56.34 | -61.91 | 5.57 |
| A:LEU\_164 | -34.12 | -40.3 | 6.18 |
| A:SER\_162 | -28.88 | -35.54 | 6.66 |
| A:PRO\_191 | -17.37 | -24.03 | 6.66 |
| A:ARG\_158 | -65.67 | -73.42 | 7.75 |
| A:ASN\_167 | -62.61 | -70.68 | 8.07 |
| A:PRO\_155 | -8.34 | -18.27 | 9.93 |
| A:GLN\_170 | -61.87 | -77.37 | 15.5 |
| A:GLN\_169 | -63.81 | -80.44 | 16.63 |
| A:LEU\_168 | -25.41 | -46.05 | 20.64 |

Physical interpretation of change in energy

|  |  |  |
| --- | --- | --- |
| **Residue(i)-Closed** | **Interaction** | **Residue(j)-Closed** |
| A:157:\_:PHE | VDW:MC\_MC | A:163:\_:GLY |
| A:157:\_:PHE | VDW:SC\_SC | A:164:\_:LEU |
| A:157:\_:PHE | HBOND:MC\_MC | A:165:\_:TYR |
| A:157:\_:PHE | PIPISTACK:SC\_SC | A:165:\_:TYR |
| A:157:\_:PHE | VDW:SC\_SC | A:165:\_:TYR |
| A:157:\_:PHE | PIPISTACK:SC\_SC | A:180:\_:PHE |
| A:157:\_:PHE | VDW:SC\_SC | A:180:\_:PHE |
| A:158:\_:ARG | VDW:SC\_SC | A:323:\_:GLU |
| A:163:\_:GLY | HBOND:MC\_MC | A:166:\_:SER |
| A:163:\_:GLY | HBOND:MC\_MC | A:167:\_:ASN |
| A:164:\_:LEU | VDW:SC\_SC | A:168:\_:LEU |
| A:164:\_:LEU | VDW:SC\_SC | A:171:\_:TYR |
| A:168:\_:LEU | HBOND:MC\_MC | A:171:\_:TYR |
| A:168:\_:LEU | VDW:SC\_SC | A:171:\_:TYR |
| A:171:\_:TYR | HBOND:SC\_SC | A:198:\_:GLU |
| A:191:\_:PRO | HBOND:MC\_MC | A:194:\_:THR |
| A:191:\_:PRO | HBOND:MC\_MC | A:195:\_:LEU |
| A:194:\_:THR | HBOND:MC\_MC | A:197:\_:LYS |
| A:194:\_:THR | HBOND:MC\_MC | A:198:\_:GLU |
| A:199:\_:LEU | VDW:SC\_SC | A:230:\_:ILE |

|  |  |  |
| --- | --- | --- |
| **Residue(i)-Open** | **Interaction** | **Residue(j)-Open** |
| A:155:\_:PRO | HBOND:MC\_MC | A:158:\_:ARG |
| A:155:\_:PRO | VDW:SC\_MC | A:158:\_:ARG |
| A:155:\_:PRO | VDW:SC\_SC | A:160:\_:PRO |
| A:155:\_:PRO | VDW:SC\_SC | A:164:\_:LEU |
| A:157:\_:PHE | VDW:SC\_SC | A:160:\_:PRO |
| A:157:\_:PHE | VDW:SC\_SC | A:176:\_:PRO |
| A:158:\_:ARG | VDW:SC\_SC | A:164:\_:LEU |
| A:158:\_:ARG | VDW:SC\_SC | A:195:\_:LEU |
| A:158:\_:ARG | IONIC:SC\_SC | A:231:\_:ASP |
| A:158:\_:ARG | HBOND:SC\_SC | A:231:\_:ASP |
| A:158:\_:ARG | VDW:SC\_SC | A:231:\_:ASP |
| A:160:\_:PRO | VDW:MC\_SC | A:165:\_:TYR |
| A:162:\_:SER | HBOND:MC\_MC | A:165:\_:TYR |
| A:162:\_:SER | HBOND:MC\_MC | A:166:\_:SER |
| A:163:\_:GLY | HBOND:MC\_MC | A:166:\_:SER |
| A:163:\_:GLY | HBOND:MC\_MC | A:167:\_:ASN |
| A:164:\_:LEU | HBOND:MC\_MC | A:167:\_:ASN |
| A:164:\_:LEU | HBOND:MC\_MC | A:168:\_:LEU |
| A:164:\_:LEU | VDW:SC\_SC | A:168:\_:LEU |
| A:164:\_:LEU | VDW:SC\_SC | A:195:\_:LEU |
| A:164:\_:LEU | VDW:SC\_SC | A:198:\_:GLU |
| A:167:\_:ASN | VDW:MC\_SC | A:170:\_:GLN |
| A:167:\_:ASN | VDW:SC\_SC | A:194:\_:THR |
| A:168:\_:LEU | HBOND:MC\_MC | A:171:\_:TYR |
| A:168:\_:LEU | VDW:MC\_SC | A:171:\_:TYR |
| A:168:\_:LEU | VDW:SC\_SC | A:173:\_:LEU |
| A:168:\_:LEU | VDW:SC\_SC | A:179:\_:ILE |
| A:168:\_:LEU | VDW:SC\_MC | A:191:\_:PRO |
| A:168:\_:LEU | VDW:SC\_SC | A:194:\_:THR |
| A:169:\_:GLN | HBOND:MC\_MC | A:172:\_:ASP |
| A:169:\_:GLN | VDW:SC\_MC | A:172:\_:ASP |
| A:169:\_:GLN | HBOND:SC\_MC | A:173:\_:LEU |
| A:169:\_:GLN | VDW:SC\_SC | A:173:\_:LEU |
| A:171:\_:TYR | VDW:SC\_SC | A:188:\_:ASN |
| A:171:\_:TYR | VDW:SC\_SC | A:190:\_:LYS |
| A:171:\_:TYR | VDW:SC\_SC | A:191:\_:PRO |
| A:171:\_:TYR | HBOND:SC\_SC | A:194:\_:THR |
| A:171:\_:TYR | VDW:SC\_SC | A:194:\_:THR |
| A:191:\_:PRO | HBOND:MC\_MC | A:195:\_:LEU |
| A:192:\_:PHE | HBOND:MC\_MC | A:195:\_:LEU |
| A:194:\_:THR | HBOND:MC\_MC | A:197:\_:LYS |
| A:194:\_:THR | HBOND:MC\_MC | A:198:\_:GLU |
| A:199:\_:LEU | VDW:SC\_SC | A:230:\_:ILE |

**Sirt3/Product Complex**

Residues with significant energy change between conformations

|  |  |  |  |
| --- | --- | --- | --- |
| **RESID** | **Open** | **Closed** | **Delta** |
| A:SER\_159 | -15.31 | -25.79 | -10.48 |
| A:ARG\_139 | -71.03 | -81.3 | -10.27 |
| A:ASP\_156 | -56.31 | -66.42 | -10.11 |
| A:ASP\_313 | -71.28 | -80.78 | -9.5 |
| A:PHE\_157 | -31.93 | -40.74 | -8.81 |
| A:GLU\_177 | -49.57 | -57.78 | -8.21 |
| A:HIE\_248 | -51.43 | -57.21 | -5.78 |
| A:ARG\_158 | -66.03 | -70.94 | -4.91 |
| A:THR\_250 | -40.82 | -45.55 | -4.73 |
| A:ASP\_172 | -59.87 | -64.54 | -4.67 |
| A:GLY\_161 | -29.55 | -33.79 | -4.24 |
| A:PRO\_155 | -16.49 | -11.52 | 4.97 |
| A:ASP\_127 | -74.63 | -69.62 | 5.01 |
| A:ASN\_167 | -71.14 | -65.8 | 5.34 |
| A:TYR\_171 | -46.64 | -41.05 | 5.59 |
| A:GLN\_170 | -73.89 | -67.13 | 6.76 |
| A:LEU\_168 | -45.04 | -36.51 | 8.53 |
| A:GLN\_169 | -76.03 | -65.22 | 10.81 |

Physical interpretation of change in energy

|  |  |  |
| --- | --- | --- |
| **RESIDUE (I) open** | **Interaction** | **RESIDUE (J) open** |
| A:127:\_:ASP | HBOND:MC\_MC | A:130:\_:GLU |
| A:127:\_:ASP | HBOND:MC\_MC | A:131:\_:LEU |
| A:139:\_:ARG | HBOND:SC\_MC | A:311:\_:MET |
| A:139:\_:ARG | HBOND:MC\_SC | A:313:\_:ASP |
| A:139:\_:ARG | VDW:SC\_SC | A:313:\_:ASP |
| A:139:\_:ARG | HBOND:MC\_MC | A:314:\_:LEU |
| A:155:\_:PRO | VDW:SC\_SC | A:160:\_:PRO |
| A:155:\_:PRO | VDW:SC\_SC | A:164:\_:LEU |
| A:158:\_:ARG | VDW:SC\_SC | A:165:\_:TYR |
| A:158:\_:ARG | VDW:SC\_SC | A:168:\_:LEU |
| A:158:\_:ARG | VDW:SC\_SC | A:176:\_:PRO |
| A:167:\_:ASN | VDW:SC\_SC | A:194:\_:THR |
| A:168:\_:LEU | HBOND:MC\_MC | A:171:\_:TYR |
| A:168:\_:LEU | HBOND:MC\_MC | A:172:\_:ASP |
| A:168:\_:LEU | VDW:SC\_SC | A:173:\_:LEU |
| A:168:\_:LEU | VDW:SC\_SC | A:179:\_:ILE |
| A:168:\_:LEU | VDW:SC\_SC | A:194:\_:THR |
| A:171:\_:TYR | VDW:SC\_SC | A:190:\_:LYS |
| A:171:\_:TYR | VDW:SC\_SC | A:191:\_:PRO |
| A:177:\_:GLU | HBOND:MC\_MC | A:180:\_:PHE |
| A:177:\_:GLU | VDW:SC\_SC | A:294:\_:PHE |
| A:248:\_:HIS | HBOND:MC\_MC | A:292:\_:VAL |
| A:248:\_:HIS | VDW:MC\_SC | A:292:\_:VAL |
| A:248:\_:HIS | VDW:SC\_SC | A:324:\_:VAL |
| A:248:\_:HIS | PIPISTACK:SC\_SC | A:327:\_:PHE |
| A:250:\_:THR | HBOND:MC\_MC | A:290:\_:ASP |
| A:250:\_:THR | VDW:MC\_SC | A:291:\_:ILE |
| A:313:\_:ASP | VDW:MC\_SC | A:338:\_:VAL |
| A:314:\_:LEU | VDW:MC\_SC | A:338:\_:VAL |

|  |  |  |
| --- | --- | --- |
| **RESIDUE (I) closed** | **Interaction** | **RESIDUE (J)closed** |
| **A:127:\_:ASP** | **HBOND:MC\_MC** | **A:130:\_:GLU** |
| **A:127:\_:ASP** | **HBOND:MC\_MC** | **A:131:\_:LEU** |
| **A:127:\_:ASP** | **VDW:MC\_SC** | **A:131:\_:LEU** |
| **A:139:\_:ARG** | **VDW:SC\_SC** | **A:311:\_:MET** |
| **A:139:\_:ARG** | **IONIC:SC\_SC** | **A:313:\_:ASP** |
| **A:139:\_:ARG** | **HBOND:SC\_SC** | **A:313:\_:ASP** |
| **A:139:\_:ARG** | **HBOND:MC\_MC** | **A:314:\_:LEU** |
| **A:156:\_:ASP** | **HBOND:SC\_SC** | **A:159:\_:SER** |
| **A:156:\_:ASP** | **VDW:SC\_SC** | **A:159:\_:SER** |
| **A:156:\_:ASP** | **HBOND:MC\_MC** | **A:164:\_:LEU** |
| **A:157:\_:PHE** | **VDW:SC\_SC** | **A:164:\_:LEU** |
| **A:157:\_:PHE** | **HBOND:MC\_MC** | **A:165:\_:TYR** |
| **A:157:\_:PHE** | **PIPISTACK:SC\_SC** | **A:165:\_:TYR** |
| **A:157:\_:PHE** | **VDW:SC\_SC** | **A:165:\_:TYR** |
| **A:157:\_:PHE** | **VDW:SC\_SC** | **A:180:\_:PHE** |
| **A:158:\_:ARG** | **VDW:SC\_SC** | **A:323:\_:GLU** |
| **A:159:\_:SER** | **HBOND:MC\_MC** | **A:163:\_:GLY** |
| **A:161:\_:GLY** | **HBOND:MC\_SC** | **A:166:\_:SER** |
| **A:168:\_:LEU** | **HBOND:MC\_MC** | **A:171:\_:TYR** |
| **A:168:\_:LEU** | **VDW:SC\_SC** | **A:171:\_:TYR** |
| **A:168:\_:LEU** | **VDW:SC\_SC** | **A:173:\_:LEU** |
| **A:171:\_:TYR** | **VDW:SC\_SC** | **A:179:\_:ILE** |
| **A:171:\_:TYR** | **VDW:SC\_SC** | **A:194:\_:THR** |
| **A:171:\_:TYR** | **HBOND:SC\_SC** | **A:198:\_:GLU** |
| **A:248:\_:HIS** | **HBOND:MC\_MC** | **A:292:\_:VAL** |
| **A:248:\_:HIS** | **VDW:MC\_SC** | **A:292:\_:VAL** |
| **A:248:\_:HIS** | **VDW:SC\_SC** | **A:324:\_:VAL** |
| **A:248:\_:HIS** | **PIPISTACK:SC\_SC** | **A:327:\_:PHE** |
| **A:250:\_:THR** | **HBOND:MC\_MC** | **A:290:\_:ASP** |
| **A:250:\_:THR** | **VDW:MC\_SC** | **A:291:\_:ILE** |
| **A:313:\_:ASP** | **HBOND:SC\_SC** | **A:335:\_:ARG** |
| **A:313:\_:ASP** | **VDW:MC\_SC** | **A:338:\_:VAL** |