**Table S1**: Frustration analysis in WT and Q94E POT1. Frustration values were calculated according to single residual frustration index level as minimally frustrated (**>0.78**) and highly frustrated (**<-0.78**).

|  |  |  |
| --- | --- | --- |
| **S. No.** | **Residue No.** | **Frustration values** |
| **WT** | **Q94E** |
|  | 6 | -0.81 | 0.514 |
|  | 7 | -0.753 | -0.056 |
|  | 8 | 0.346 | 1.148 |
|  | 9 | -2.159 | -1.141 |
|  | 10 | 0.712 | -0.007 |
|  | 11 | 1.169 | 1.163 |
|  | 12 | -0.154 | -0.26 |
|  | 13 | -1.47 | -1.677 |
|  | 14 | 1.138 | 1.177 |
|  | 15 | -0.908 | -0.99 |
|  | 16 | -0.631 | -0.293 |
|  | 17 | 1.176 | 1.33 |
|  | 18 | -0.509 | -0.135 |
|  | 19 | -0.382 | -0.498 |
|  | 20 | -0.584 | -0.806 |
|  | 21 | -0.19 | -0.17 |
|  | 22 | 1.034 | 0.958 |
|  | 23 | 1.252 | 1.186 |
|  | 24 | -0.99 | -1.107 |
|  | 25 | 1.191 | 1.28 |
|  | 26 | 0.768 | 0.593 |
|  | 27 | -0.519 | -0.468 |
|  | 28 | 1.253 | 1.279 |
|  | 29 | 1.221 | 1.193 |
|  | 30 | -1.545 | -1.637 |
|  | 31 | 0.89 | 1.425 |
|  | 32 | 1.063 | 1.238 |
|  | 33 | -1.539 | -1.906 |
|  | 34 | -1.138 | -1.111 |
|  | 35 | -0.827 | -0.823 |
|  | 36 | 1.558 | 0.835 |
|  | 37 | -0.564 | 0.465 |
|  | 38 | -0.182 | -0.668 |
|  | 39 | 0.031 | -0.3 |
|  | 40 | -0.537 | -0.484 |
|  | 41 | 0.061 | 0.043 |
|  | 42 | -1.522 | -0.948 |
|  | 43 | 0.737 | 0.654 |
|  | 44 | 1.545 | 1.297 |
|  | 45 | -0.753 | -0.708 |
|  | 46 | 1.291 | 1.321 |
|  | 47 | 1.094 | 1.113 |
|  | 48 | -0.549 | -0.485 |
|  | 49 | 1.382 | 1.358 |
|  | 50 | 1.063 | 1.189 |
|  | 51 | -1.058 | -1.086 |
|  | 52 | -0.78 | -0.866 |
|  | 53 | -0.262 | 0.145 |
|  | 54 | -1.466 | 0.174 |
|  | 55 | 1.15 | 1.212 |
|  | 56 | -1.567 | -0.869 |
|  | 57 | 1.166 | 1.288 |
|  | 58 | -0.066 | 0.115 |
|  | 59 | 1.076 | 1.43 |
|  | 60 | 1.249 | 0.968 |
|  | 61 | 1.13 | 1.127 |
|  | 62 | 1.044 | 1.087 |
|  | 63 | -0.512 | -0.577 |
|  | 64 | -0.338 | -0.347 |
|  | 65 | -0.423 | -0.813 |
|  | 66 | 0.227 | 0.388 |
|  | 67 | -1.809 | -1.648 |
|  | 68 | 0.032 | 0.067 |
|  | 69 | 0.936 | 0.992 |
|  | 70 | -1.141 | -1.053 |
|  | 71 | 1.498 | 1.848 |
|  | 72 | 1.224 | 1.292 |
|  | 73 | 1.009 | -1.169 |
|  | 74 | -0.043 | -0.891 |
|  | 75 | -0.982 | -1.028 |
|  | 76 | -0.337 | -0.415 |
|  | 77 | -1.4 | -1.371 |
|  | 78 | 1.49 | 1.492 |
|  | 79 | 1.306 | 1.267 |
|  | 80 | -0.841 | -0.702 |
|  | 81 | 1.294 | 1.172 |
|  | 82 | -0.499 | -0.235 |
|  | 83 | -0.699 | -0.704 |
|  | 84 | 1.406 | 1.381 |
|  | 85 | -1.66 | -1.594 |
|  | 86 | 1.398 | 1.437 |
|  | 87 | -1.084 | -1.157 |
|  | 88 | 0.264 | 0.808 |
|  | 89 | -1.892 | -2.559 |
|  | 90 | 1.033 | 1.684 |
|  | 91 | -1.381 | -1.271 |
|  | 92 | -0.52 | 0.935 |
|  | 93 | -0.363 | -0.353 |
|  | 94 | -0.958 | -0.972 |
|  | 95 | -0.558 | -0.439 |
|  | 96 | 1.578 | 1.48 |
|  | 97 | -0.315 | -0.402 |
|  | 98 | -0.812 | -0.843 |
|  | 99 | 0.122 | -0.521 |
|  | 100 | -0.046 | -0.594 |
|  | 101 | 1.098 | 1.415 |
|  | 102 | 0.046 | -0.884 |
|  | 103 | -0.72 | -0.638 |
|  | 104 | 1.079 | 1.145 |
|  | 105 | -0.27 | -0.203 |
|  | 106 | 1.234 | 1.08 |
|  | 107 | 0.385 | -1.152 |
|  | 108 | -0.384 | -0.437 |
|  | 109 | 0.654 | 0.511 |
|  | 110 | 0.705 | -0.334 |
|  | 111 | 0.049 | -0.409 |
|  | 112 | -0.017 | 0.412 |
|  | 113 | -0.192 | -0.512 |
|  | 114 | 1.405 | 1.124 |
|  | 115 | 1.664 | 1.404 |
|  | 116 | -1.149 | -0.983 |
|  | 117 | -0.315 | -0.897 |
|  | 118 | -0.248 | -0.12 |
|  | 119 | -0.224 | -0.474 |
|  | 120 | -0.893 | -0.863 |
|  | 121 | -0.738 | -0.729 |
|  | 122 | -2.25 | -2.497 |
|  | 123 | 1.004 | 1.245 |
|  | 124 | -0.711 | -0.549 |
|  | 125 | 0.909 | 1.135 |
|  | 126 | 0.725 | 1.021 |
|  | 127 | 0.994 | 0.612 |
|  | 128 | -0.502 | -0.132 |
|  | 129 | -1.212 | -1.181 |
|  | 130 | -0.227 | -0.203 |
|  | 131 | 1.64 | 0.026 |
|  | 132 | 0.897 | 1.017 |
|  | 133 | 1.28 | 1.329 |
|  | 134 | -0.678 | -0.753 |
|  | 135 | 0.476 | 0.415 |
|  | 136 | 1.252 | 1.201 |
|  | 137 | -0.746 | -0.761 |
|  | 138 | 1.359 | 1.301 |
|  | 139 | 0.373 | 0.374 |
|  | 140 | 0.722 | 0.571 |
|  | 141 | -0.712 | -0.578 |
|  | 142 | -0.267 | -0.494 |
|  | 143 | -0.132 | -0.466 |
|  | 144 | 0.793 | -0.171 |
|  | 145 | 0.017 | -1.005 |
|  | 146 | -1.257 | -1.212 |
|  | 147 | -0.285 | -0.566 |
|  | 148 | -1.678 | -2.077 |
|  | 149 | -0.156 | -0.144 |
|  | 150 | 1.175 | 1.36 |
|  | 151 | 1.427 | 1.451 |
|  | 152 | -0.74 | -1.363 |
|  | 153 | 1.255 | 1.383 |
|  | 154 | 0.663 | 2.212 |
|  | 155 | -0.019 | -1.053 |
|  | 156 | 1.327 | 1.259 |
|  | 157 | -0.885 | -0.769 |
|  | 158 | -0.849 | -0.944 |
|  | 159 | -1.079 | 0.682 |
|  | 160 | -0.632 | 0.038 |
|  | 161 | -0.661 | 0.187 |
|  | 162 | 1.137 | 1.2 |
|  | 163 | -0.954 | -1.052 |
|  | 164 | 1.385 | 1.376 |
|  | 165 | -0.262 | -0.228 |
|  | 166 | 0.709 | 0.637 |
|  | 167 | -0.902 | -0.876 |
|  | 168 | 1.049 | 1.196 |
|  | 169 | 1.317 | 1.356 |
|  | 170 | -0.641 | -0.553 |
|  | 171 | -1.105 | -1.129 |
|  | 172 | 0.927 | 0.429 |
|  | 173 | -1.28 | -1.295 |
|  | 174 | 1.452 | 1.296 |
|  | 175 | -1.06 | -1.155 |
|  | 176 | -0.597 | -0.309 |
|  | 177 | 0.147 | -0.065 |
|  | 178 | -0.644 | -0.672 |
|  | 179 | 1.259 | 1.256 |
|  | 180 | 1.252 | 1.195 |
|  | 181 | 1.424 | 1.416 |
|  | 182 | -1.111 | -1.029 |
|  | 183 | 1.046 | 1.081 |
|  | 184 | 0.478 | 0.553 |
|  | 185 | -1.388 | -1.121 |
|  | 186 | -0.486 | -0.4 |
|  | 187 | -0.342 | -0.102 |
|  | 188 | -0.222 | 0.011 |
|  | 189 | -0.315 | -0.232 |
|  | 190 | -1.011 | -1.322 |
|  | 191 | 1.004 | 1.095 |
|  | 192 | -0.845 | -1.219 |
|  | 193 | -0.701 | -0.624 |
|  | 194 | 0.865 | 0.711 |
|  | 195 | 0.758 | 1.219 |
|  | 196 | 1.289 | 1.193 |
|  | 197 | -0.698 | -0.027 |
|  | 198 | 1.377 | 1.352 |
|  | 199 | -0.876 | -0.855 |
|  | 200 | -1.353 | -1.339 |
|  | 201 | 1.617 | 1.344 |
|  | 202 | 1.278 | 0.702 |
|  | 203 | 1.259 | 1.573 |
|  | 204 | -0.762 | -1.229 |
|  | 205 | -0.741 | -0.393 |
|  | 206 | -0.819 | -0.886 |
|  | 207 | 0.741 | 1.138 |
|  | 208 | 0.334 | 0.037 |
|  | 209 | -0.283 | -0.093 |
|  | 210 | 1.249 | 1.148 |
|  | 211 | -0.171 | -0.477 |
|  | 212 | -1.049 | -0.654 |
|  | 213 | 1.35 | 1.299 |
|  | 214 | -1.067 | -1.068 |
|  | 215 | 0.377 | 0.066 |
|  | 216 | 1.323 | 1.447 |
|  | 217 | -0.362 | -0.346 |
|  | 218 | 1.407 | 1.367 |
|  | 219 | -1.142 | -1.02 |
|  | 220 | 1.429 | 1.442 |
|  | 221 | 1.136 | 1.136 |
|  | 222 | 1.174 | 1.221 |
|  | 223 | 0.903 | 0.742 |
|  | 224 | -0.641 | -1.063 |
|  | 225 | -0.734 | -0.649 |
|  | 226 | -0.184 | -0.21 |
|  | 227 | 1.448 | 1.477 |
|  | 228 | -0.358 | 0.618 |
|  | 229 | 1.356 | 1.256 |
|  | 230 | 0.485 | 0.551 |
|  | 231 | -0.776 | -0.755 |
|  | 232 | -0.693 | -1.169 |
|  | 233 | 1.333 | 1.345 |
|  | 234 | -1.29 | -1.608 |
|  | 235 | 0.919 | 1.027 |
|  | 236 | -0.881 | -0.639 |
|  | 237 | -0.792 | -0.729 |
|  | 238 | 0.933 | 0.96 |
|  | 239 | 1.319 | 1.284 |
|  | 240 | -0.63 | -0.54 |
|  | 241 | 1.234 | 1.321 |
|  | 242 | 0.646 | 0.761 |
|  | 243 | -0.681 | -0.711 |
|  | 244 | 1.225 | 1.198 |
|  | 245 | 0.525 | 0.228 |
|  | 246 | -0.258 | -0.233 |
|  | 247 | -0.889 | -0.689 |
|  | 248 | 1.166 | 1.175 |
|  | 249 | -1.024 | -1.126 |
|  | 250 | -0.723 | -0.854 |
|  | 251 | 0.678 | -1.691 |
|  | 252 | -0.983 | -0.985 |
|  | 253 | -0.774 | -0.389 |
|  | 254 | -0.061 | 0.94 |
|  | 255 | 0.929 | -0.203 |
|  | 256 | -0.819 | 0.139 |
|  | 257 | 1.01 | -0.137 |
|  | 258 | -0.735 | -2.733 |
|  | 259 | 1.133 | 1.109 |
|  | 260 | -0.598 | -0.605 |
|  | 261 | 1.274 | 1.366 |
|  | 262 | -0.985 | -0.965 |
|  | 263 | 1.255 | 1.233 |
|  | 264 | -0.305 | -0.273 |
|  | 265 | 1.361 | 1.321 |
|  | 266 | 0.322 | 0.063 |
|  | 267 | -0.373 | 0.046 |
|  | 268 | 0.759 | -0.282 |
|  | 269 | 0.246 | -0.468 |
|  | 270 | 0.745 | -0.648 |
|  | 271 | -2.519 | 1.441 |
|  | 272 | -0.18 | 0.787 |
|  | 273 | -0.595 | -0.604 |
|  | 274 | -0.411 | -0.31 |
|  | 275 | 1.343 | 1.487 |
|  | 276 | -0.772 | -0.757 |
|  | 277 | 1.192 | 1.091 |
|  | 278 | 1.047 | 1.054 |
|  | 279 | -1.822 | -1.603 |
|  | 280 | -1.395 | -1.195 |
|  | 281 | -0.886 | -0.597 |
|  | 282 | -1.021 | -0.788 |
|  | 283 | 0.475 | 0.971 |
|  | 284 | -1.021 | -1.004 |
|  | 285 | 1.114 | 1.237 |
|  | 286 | 2.088 | 0.499 |
|  | 287 | -0.231 | -0.036 |
|  | 288 | 0.806 | 0.897 |
|  | 289 | -0.957 | -0.701 |
|  | 290 | 0.664 | -0.637 |
|  | 291 | -1.203 | -1.222 |
|  | 292 | 0.918 | 1.298 |
|  | 293 | 1.076 | 0.898 |
|  | 294 | -0.522 | -0.617 |
|  | 295 | -0.141 | 0.569 |
|  | 296 | -1.043 | -0.905 |
|  | 297 | -0.429 | -0.984 |
|  | 298 | 0.033 | 0.34 |
|  | 299 | 0.788 | 0.578 |
|  | 300 | 0.16 | -0.426 |