Hydrogen bonds observed during last 400ns of MD simulations between h FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|--------------------------------|---------|-----------------------------------|
| 27        | OH           | O4         | 66                        | 0.330%                         | 0       | 1.310%                            |
| 27        | OH           | O5         | 195                       | 0.975%                         | 0       |                                   |
| 27        | OH           | O6         | 1                         | 0.005%                         | 0       | 0.005%                            |
| 29        | N            | O6         | 1                         | 0.005%                         | 0       | 0.005%                            |
| 37        | O            | O6         | 32                        | 0.160%                         | 0       | 0.160%                            |
| 38        | N            | O4         | 11                        | 0.055%                         | 0       |                                   |
| 38        | N            | O6         | 500                       | 2.499%                         | 0       |                                   |
| 38        | OD1          | O4         | 14                        | 0.070%                         | 0       |                                   |
| 38        | OD1          | O5         | 123                       | 0.615%                         | 0       |                                   |
| 38        | OD1          | O6         | 358                       | 1.790%                         | 0       |                                   |
| 38        | OD1          | O7         | 4                         | 0.020%                         | 0       |                                   |
| 38        | OD2          | O4         | 14                        | 0.070%                         | 0       | 21.800%                           |
| 38        | OD2          | O5         | 151                       | 0.755%                         | 0       |                                   |
| 38        | OD2          | O6         | 392                       | 1.960%                         | 0       |                                   |
| 38        | O            | O4         | 739                       | 3.694%                         | 0       |                                   |
| 38        | O            | O5         | 41                        | 0.205%                         | 0       |                                   |
| 38        | O            | O6         | 2013                      | 10.063%                        | 1       |                                   |
| 43        | NH1          | O5         | 1                         | 0.005%                         | 0       |                                   |
| 43        | NH1          | O6         | 49                        | 0.245%                         | 0       |                                   |
| 43        | NH1          | O7         | 4                         | 0.020%                         | 0       |                                   |
| 43        | NH1          | O8         | 87                        | 0.435%                         | 0       |                                   |
| 43        | NH2          | O4         | 76                        | 0.380%                         | 0       | 1.445%                            |
| 43        | NH2          | O5         | 56                        | 0.280%                         | 0       |                                   |
| 43        | NH2          | O6         | 1                         | 0.005%                         | 0       |                                   |
| 43        | NH2          | O7         | 1                         | 0.005%                         | 0       |                                   |
| 43        | NH2          | O8         | 14                        | 0.070%                         | 0       |                                   |
| 44        | ND2          | O6         | 1                         | 0.005%                         | 0       | 0.005%                            |
| 53        | NZ           | O10        | 5                         | 0.025%                         | 0       | 0.025%                            |
| 54        | NE2          | O10        | 1                         | 0.005%                         | 0       |                                   |
| 54        | NE2          | O11        | 5                         | 0.025%                         | 0       |                                   |
| 54        | NE2          | O12        | 9                         | 0.045%                         | 0       |                                   |
| 54        | OE1          | O11        | 1                         | 0.005%                         | 0       | 0.350%                            |
| 54        | OE1          | O12        | 4                         | 0.020%                         | 0       |                                   |
| 54        | O            | O10        | 1                         | 0.005%                         | 0       |                                   |
| 54        | O            | O11        | 33                        | 0.165%                         | 0       |                                   |
| 54        | O            | O12        | 16                        | 0.080%                         | 0       |                                   |
| 55        | N            | O10        | 3                         | 0.015%                         | 0       |                                   |
| 55        | OE1          | O10        | 27                        | 0.135%                         | 0       |                                   |
| 55        | OE2          | O10        | 28                        | 0.140%                         | 0       |                                   |
Hydrogen bonds observed during last 400ns of MD simulations between h FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|--------------------------|-------------------------------|---------|-----------------------------------|
| 55        | OE2          | O12         | 1                        | 0.005%                        | 0       | 34.636%                           |
| 55        | O            | O10         | 6811                     | 34.047%                       | 5       |                                   |
| 55        | O            | O11         | 32                       | 0.160%                        | 0       |                                   |
| 55        | O            | O12         | 13                       | 0.065%                        | 0       |                                   |
| 55        | O            | O2          | 14                       | 0.070%                        | 0       |                                   |
| 56        | N            | O10         | 3                        | 0.015%                        | 0       |                                   |
| 56        | O            | O11         | 94                       | 0.470%                        | 0       | 0.510%                            |
| 56        | O            | O12         | 5                        | 0.025%                        | 0       |                                   |
| 57        | N            | O2          | 13660                    | 68.283%                       | 9       | 68.283%                           |
| 58        | NH1          | O11         | 19                       | 0.095%                        | 0       |                                   |
| 58        | NH2          | O11         | 2                        | 0.010%                        | 0       | 0.105%                            |
| 60        | NE1          | O11         | 2131                     | 10.652%                       | 1       |                                   |
| 60        | NE1          | O12         | 17                       | 0.085%                        | 0       |                                   |
| 60        | NE1          | O2          | 5                        | 0.025%                        | 0       | 30.542%                           |
| 60        | NE1          | O3          | 3940                     | 19.695%                       | 3       |                                   |
| 60        | NE1          | O4          | 15                       | 0.075%                        | 0       |                                   |
| 60        | N            | O12         | 2                        | 0.010%                        | 0       |                                   |
| 79        | O            | O12         | 124                      | 0.620%                        | 0       | 0.620%                            |
| 82        | O            | O11         | 16                       | 0.080%                        | 0       | 0.230%                            |
| 82        | O            | O12         | 30                       | 0.150%                        | 0       |                                   |
| 83        | N            | O11         | 1                        | 0.005%                        | 0       |                                   |
| 83        | N            | O12         | 14                       | 0.070%                        | 0       |                                   |
| 83        | OH           | O10         | 6                        | 0.030%                        | 0       |                                   |
| 83        | OH           | O11         | 74                       | 0.370%                        | 0       | 2.579%                            |
| 83        | OH           | O12         | 306                      | 1.530%                        | 0       |                                   |
| 83        | OH           | O3          | 3                        | 0.015%                        | 0       |                                   |
| 83        | O            | O11         | 9                        | 0.045%                        | 0       |                                   |
| 83        | O            | O12         | 103                      | 0.515%                        | 0       |                                   |
| 84        | N            | O11         | 1658                     | 8.288%                        | 1       |                                   |
| 84        | N            | O12         | 234                      | 1.170%                        | 0       | 10.972%                           |
| 84        | O            | O11         | 146                      | 0.730%                        | 0       |                                   |
| 84        | O            | O12         | 157                      | 0.785%                        | 0       |                                   |
| 85        | N            | O11         | 699                      | 3.494%                        | 0       |                                   |
| 85        | N            | O12         | 297                      | 1.485%                        | 0       | 12.787%                           |
| 85        | O            | O11         | 93                       | 0.465%                        | 0       |                                   |
| 85        | O            | O12         | 1469                     | 7.343%                        | 1       |                                   |
| 86        | N            | O11         | 438                      | 2.189%                        | 0       |                                   |
| 86        | N            | O12         | 309                      | 1.545%                        | 0       |                                   |
| 86        | OG1          | O11         | 567                      | 2.834%                        | 0       |                                   |
| 86        | OG1          | O12         | 885                      | 4.424%                        | 0       | 12.617%                           |
Hydrogen bonds observed during last 400ns of MD simulations between hFKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 86        | O            | O10         | 1                         | 0.005%                        | 0       |
| 86        | O            | O11         | 24                        | 0.120%                        | 0       |
| 86        | O            | O12         | 300                       | 1.500%                        | 0       |
| 87        | N            | O11         | 89                        | 0.445%                        | 0       |
| 87        | N            | O12         | 283                       | 1.415%                        | 0       |
| 87        | O            | O10         | 1                         | 0.005%                        | 0       |
| 87        | O            | O11         | 29                        | 0.145%                        | 0       |
| 87        | O            | O12         | 368                       | 1.840%                        | 0       |
| 88        | ND1          | O10         | 7                         | 0.035%                        | 0       |
| 88        | ND1          | O12         | 54                        | 0.270%                        | 0       |
| 88        | ND1          | O9          | 1                         | 0.005%                        | 0       |
| 88        | NE2          | O10         | 254                       | 1.270%                        | 0       |
| 88        | NE2          | O11         | 50                        | 0.250%                        | 0       |
| 88        | NE2          | O12         | 47                        | 0.235%                        | 0       |
| 88        | NE2          | O9          | 71                        | 0.355%                        | 1       |
| 88        | N            | O10         | 2                         | 0.010%                        | 0       |
| 88        | N            | O11         | 59                        | 0.295%                        | 0       |
| 88        | N            | O12         | 466                       | 2.329%                        | 0       |
| 88        | N            | O9          | 2                         | 0.010%                        | 0       |
| 88        | O            | O10         | 40                        | 0.200%                        | 0       |
| 88        | O            | O11         | 62                        | 0.310%                        | 0       |
| 88        | O            | O12         | 1258                      | 6.288%                        | 0       |
| 88        | O            | O9          | 22                        | 0.110%                        | 0       |
| 89        | N            | O11         | 3                         | 0.015%                        | 0       |
| 89        | N            | O12         | 6                         | 0.030%                        | 0       |
| 89        | O            | O10         | 122                       | 0.610%                        | 0       |
| 89        | O            | O11         | 13                        | 0.065%                        | 0       |
| 89        | O            | O12         | 31                        | 0.155%                        | 0       |
| 89        | O            | O7          | 3                         | 0.015%                        | 0       |
| 89        | O            | O9          | 50                        | 0.250%                        | 0       |
| 90        | N            | O11         | 19                        | 0.095%                        | 0       |
| 90        | N            | O12         | 125                       | 0.625%                        | 0       |
| 90        | N            | O7          | 4                         | 0.020%                        | 0       |
| 90        | N            | O9          | 32                        | 0.160%                        | 0       |
| 90        | O            | O11         | 11                        | 0.055%                        | 0       |
| 90        | O            | O12         | 9                         | 0.045%                        | 0       |
| 90        | O            | O7          | 3                         | 0.015%                        | 0       |
| 90        | O            | O9          | 1                         | 0.005%                        | 0       |
| 91        | N            | O11         | 15                        | 0.075%                        | 0       |
| 91        | N            | O12         | 1                         | 0.005%                        | 0       |
| 91        | N            | O7          | 282                       | 1.410%                        | 0       |
Hydrogen bonds observed during last 400ns of MD simulations between h FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 91        | N            | O9         | 1178                      | 5.889%                        | 1       | 7.478%                            |
| 91        | O            | O12        | 11                        | 0.055%                        | 0       |                                   |
| 91        | O            | O3         | 1                         | 0.005%                        | 0       |                                   |
| 91        | O            | O7         | 7                         | 0.035%                        | 0       |                                   |
| 91        | O            | O9         | 1                         | 0.005%                        | 0       |                                   |
| 93        | O            | O11        | 1                         | 0.005%                        | 0       | 0.005%                            |
| 95        | NE2          | O11        | 4                         | 0.020%                        | 0       | 0.020%                            |
Hydrogen bonds observed during last 400ns of MD simulations between h FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 27        | OH           | O4          | 14                        | 0.070%                        | 0       |                                   |
| 27        | OH           | O5          | 5                         | 0.025%                        | 0       |                                   |
| 27        | OH           | O6          | 161                       | 0.805%                        | 0       | 3.574%                           |
| 27        | OH           | O8          | 530                       | 2.649%                        | 0       |                                   |
| 27        | OH           | O13         | 5                         | 0.025%                        | 0       |                                   |
| 28        | O            | O4          | 3                         | 0.015%                        | 0       | 0.015%                           |
| 28        | O            | O6          | 3                         | 0.015%                        | 0       | 0.015%                           |
| 37        | O            | O4          | 232                       | 1.160%                        | 0       |                                   |
| 38        | N            | O4          | 1                         | 0.005%                        | 0       |                                   |
| 38        | N            | O6          | 19                        | 0.095%                        | 0       |                                   |
| 38        | N            | O8          | 3                         | 0.015%                        | 0       |                                   |
| 38        | OD1          | O4          | 113                       | 0.565%                        | 0       |                                   |
| 38        | OD1          | O6          | 3129                      | 15.641%                       | 5       |                                   |
| 38        | OD1          | O8          | 29                        | 0.145%                        | 0       |                                   |
| 38        | OD2          | O4          | 129                       | 0.645%                        | 0       | 39.745%                          |
| 38        | OD2          | O5          | 3                         | 0.015%                        | 0       |                                   |
| 38        | OD2          | O6          | 3356                      | 16.776%                       | 5       |                                   |
| 38        | OD2          | O8          | 29                        | 0.145%                        | 0       |                                   |
| 38        | O            | O4          | 232                       | 1.160%                        | 0       |                                   |
| 38        | O            | O5          | 1                         | 0.005%                        | 0       |                                   |
| 38        | O            | O6          | 907                       | 4.534%                        | 1       |                                   |
| 39        | OG           | O6          | 1                         | 0.005%                        | 0       | 0.005%                           |
| 43        | NE           | O6          | 19                        | 0.095%                        | 0       |                                   |
| 43        | NE           | O8          | 479                       | 2.394%                        | 0       |                                   |
| 43        | NE           | O13         | 10                        | 0.050%                        | 0       |                                   |
| 43        | NH1          | O4          | 523                       | 2.614%                        | 0       |                                   |
| 43        | NH1          | O5          | 746                       | 3.729%                        | 1       |                                   |
| 43        | NH1          | O6          | 868                       | 4.339%                        | 1       |                                   |
| 43        | NH1          | O7          | 3                         | 0.015%                        | 0       |                                   |
| 43        | NH1          | O8          | 2323                      | 11.612%                       | 3       |                                   |
| 43        | NH1          | O10         | 1                         | 0.005%                        | 0       | 55.281%                          |
| 43        | NH1          | O13         | 24                        | 0.120%                        | 0       |                                   |
| 43        | NH2          | N54         | 1                         | 0.005%                        | 0       |                                   |
| 43        | NH2          | O4          | 22                        | 0.110%                        | 0       |                                   |
| 43        | NH2          | O5          | 53                        | 0.265%                        | 0       |                                   |
| 43        | NH2          | O6          | 3781                      | 18.900%                       | 6       |                                   |
| 43        | NH2          | O7          | 21                        | 0.105%                        | 0       |                                   |
| 43        | NH2          | O8          | 2176                      | 10.877%                       | 3       |                                   |
| 43        | NH2          | O13         | 9                         | 0.045%                        | 0       |                                   |
Hydrogen bonds observed during last 400ns of MD simulations between hFKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 48        | O            | O11         | 2                         | 0.010%                        | 0       | 1.185%                            |
| 48        | O            | O12         | 101                       | 0.505%                        | 0       | 11.537%                           |
| 48        | O            | O13         | 110                       | 0.550%                        | 0       | 1.185%                            |
| 50        | N            | O10         | 354                       | 1.770%                        | 0       | 1.510%                            |
| 50        | N            | O11         | 4                         | 0.020%                        | 0       | 1.185%                            |
| 50        | N            | O12         | 269                       | 1.345%                        | 0       | 1.185%                            |
| 50        | N            | O13         | 1663                      | 8.313%                        | 2       | 26.458%                           |
| 50        | O            | O10         | 5                         | 0.025%                        | 0       | 1.185%                            |
| 50        | O            | O12         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 50        | O            | O13         | 12                        | 0.060%                        | 0       | 1.185%                            |
| 52        | O            | N55         | 1                         | 0.005%                        | 0       | 0.005%                            |
| 53        | NZ           | O10         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 53        | NZ           | O11         | 4                         | 0.020%                        | 0       | 1.185%                            |
| 53        | NZ           | O12         | 15                        | 0.075%                        | 0       | 1.185%                            |
| 53        | NZ           | O13         | 137                       | 0.685%                        | 0       | 1.365%                            |
| 53        | O            | N55         | 144                       | 0.720%                        | 0       | 1.185%                            |
| 53        | O            | O10         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 54        | NE2          | N55         | 4                         | 0.020%                        | 0       | 1.185%                            |
| 54        | NE2          | O10         | 14                        | 0.070%                        | 0       | 1.185%                            |
| 54        | NE2          | O11         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 54        | NE2          | O12         | 3                         | 0.015%                        | 0       | 1.185%                            |
| 54        | NE2          | O13         | 39                        | 0.195%                        | 0       | 1.185%                            |
| 54        | OE1          | N54         | 3                         | 0.015%                        | 0       | 1.185%                            |
| 54        | OE1          | N55         | 161                       | 0.805%                        | 0       | 1.365%                            |
| 54        | OE1          | O10         | 3                         | 0.015%                        | 0       | 1.185%                            |
| 54        | OE1          | O12         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 54        | OE1          | O13         | 13                        | 0.065%                        | 0       | 1.185%                            |
| 54        | O            | N55         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 54        | O            | O10         | 4                         | 0.020%                        | 0       | 1.185%                            |
| 54        | O            | O11         | 18                        | 0.090%                        | 0       | 1.185%                            |
| 54        | O            | O12         | 8                         | 0.040%                        | 0       | 1.185%                            |
| 55        | OE1          | N55         | 120                       | 0.600%                        | 0       | 1.185%                            |
| 55        | OE1          | O10         | 102                       | 0.510%                        | 0       | 1.185%                            |
| 55        | OE1          | O11         | 1                         | 0.005%                        | 0       | 1.185%                            |
| 55        | OE1          | O12         | 574                       | 2.869%                        | 1       | 26.458%                           |
| 55        | OE1          | O13         | 6                         | 0.030%                        | 0       | 1.185%                            |
| 55        | OE2          | N55         | 97                        | 0.485%                        | 0       | 1.185%                            |
| 55        | OE2          | O10         | 81                        | 0.405%                        | 0       | 1.185%                            |
| 55        | OE2          | O12         | 579                       | 2.894%                        | 1       | 26.458%                           |
| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|--------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 55        | OE2          | O13          | 4                         | 0.020%                        | 0       |                                   |
| 55        | O            | N55          | 197                       | 0.985%                        | 0       |                                   |
| 55        | O            | O2           | 61                        | 0.305%                        | 0       |                                   |
| 55        | O            | O10          | 3387                      | 16.931%                       | 5       |                                   |
| 55        | O            | O11          | 78                        | 0.390%                        | 0       |                                   |
| 55        | O            | O12          | 6                         | 0.030%                        | 0       |                                   |
| 56        | N            | O10          | 61                        | 0.305%                        | 0       |                                   |
| 56        | O            | O11          | 10                        | 0.050%                        | 0       | 0.360%                            |
| 56        | O            | O12          | 1                         | 0.005%                        | 0       |                                   |
| 57        | N            | O2           | 2567                      | 12.832%                       | 4       | 13.112%                           |
| 57        | N            | O10          | 56                        | 0.280%                        | 0       |                                   |
| 58        | NH1          | O11          | 7                         | 0.035%                        | 0       |                                   |
| 58        | NH1          | O12          | 3                         | 0.015%                        | 0       | 0.060%                            |
| 58        | NH2          | O11          | 2                         | 0.010%                        | 0       |                                   |
| 60        | NE1          | N45          | 1                         | 0.005%                        | 0       |                                   |
| 60        | NE1          | O2           | 4                         | 0.020%                        | 0       |                                   |
| 60        | NE1          | O3           | 963                       | 4.814%                        | 1       | 6.758%                            |
| 60        | NE1          | O4           | 383                       | 1.915%                        | 0       |                                   |
| 60        | NE1          | O12          | 1                         | 0.005%                        | 0       |                                   |
| 81        | OH           | O2           | 26                        | 0.130%                        | 0       |                                   |
| 81        | OH           | O3           | 30                        | 0.150%                        | 0       |                                   |
| 81        | OH           | O11          | 1                         | 0.005%                        | 0       | 0.655%                            |
| 81        | OH           | O12          | 1                         | 0.005%                        | 0       |                                   |
| 81        | O            | O11          | 7                         | 0.035%                        | 0       |                                   |
| 81        | O            | O12          | 66                        | 0.330%                        | 0       |                                   |
| 82        | O            | O3           | 1                         | 0.005%                        | 0       |                                   |
| 82        | O            | O7           | 1                         | 0.005%                        | 0       | 0.165%                            |
| 82        | O            | O11          | 1                         | 0.005%                        | 0       |                                   |
| 82        | O            | O12          | 30                        | 0.150%                        | 0       |                                   |
| 83        | OH           | O3           | 14                        | 0.070%                        | 0       |                                   |
| 83        | OH           | O11          | 9                         | 0.045%                        | 0       |                                   |
| 83        | OH           | O12          | 108                       | 0.540%                        | 0       | 1.065%                            |
| 83        | O            | O11          | 19                        | 0.095%                        | 0       |                                   |
| 83        | O            | O12          | 63                        | 0.315%                        | 0       |                                   |
| 84        | N            | O11          | 72                        | 0.360%                        | 0       |                                   |
| 84        | N            | O12          | 49                        | 0.245%                        | 0       | 1.170%                            |
| 84        | O            | O11          | 34                        | 0.170%                        | 0       |                                   |
| 84        | O            | O12          | 79                        | 0.395%                        | 0       |                                   |
| 85        | N            | O11          | 140                       | 0.700%                        | 0       |                                   |
| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-----------------------------|---------|----------------------------------|
| 85        | N            | O12         | 225                       | 1.125%                      | 0       | 9.933%                           |
| 85        | O            | O7          | 4                         | 0.020%                      | 0       | 6.353%                           |
| 85        | O            | O11         | 123                       | 0.615%                      | 0       | 1.130%                           |
| 85        | O            | O12         | 98                        | 0.490%                      | 0       | 1.130%                           |
| 86        | N            | O11         | 38                        | 0.190%                      | 0       | 9.323%                           |
| 86        | N            | O12         | 421                       | 2.104%                      | 0       |                                  |
| 86        | OG1          | O10         | 25                        | 0.125%                      | 0       |                                  |
| 86        | OG1          | O11         | 186                       | 0.930%                      | 0       |                                  |
| 86        | OG1          | O12         | 1016                      | 5.079%                      | 1       |                                  |
| 86        | O            | N55         | 14                        | 0.070%                      | 0       |                                  |
| 86        | O            | O7          | 4                         | 0.020%                      | 0       |                                  |
| 86        | O            | O10         | 25                        | 0.125%                      | 0       |                                  |
| 86        | O            | O11         | 7                         | 0.035%                      | 0       |                                  |
| 86        | O            | O12         | 123                       | 0.615%                      | 0       |                                  |
| 86        | O            | O13         | 6                         | 0.030%                      | 0       |                                  |
| 87        | N            | O7          | 53                        | 0.265%                      | 0       | 9.933%                           |
| 87        | N            | O11         | 35                        | 0.175%                      | 0       |                                  |
| 87        | N            | O12         | 1493                      | 7.463%                      | 2       |                                  |
| 87        | O            | O10         | 1                         | 0.005%                      | 0       |                                  |
| 87        | O            | O11         | 67                        | 0.335%                      | 0       |                                  |
| 87        | O            | O12         | 338                       | 1.690%                      | 0       |                                  |
| 88        | ND1          | N55         | 1                         | 0.005%                      | 0       |                                  |
| 88        | ND1          | O10         | 3                         | 0.015%                      | 0       |                                  |
| 88        | ND1          | O12         | 32                        | 0.160%                      | 0       |                                  |
| 88        | NE2          | O7          | 5                         | 0.025%                      | 0       |                                  |
| 88        | NE2          | O10         | 7                         | 0.035%                      | 0       |                                  |
| 88        | NE2          | O11         | 6                         | 0.030%                      | 0       |                                  |
| 88        | NE2          | O12         | 63                        | 0.315%                      | 0       |                                  |
| 88        | NE2          | O13         | 3                         | 0.015%                      | 0       |                                  |
| 88        | N            | O11         | 114                       | 0.570%                      | 0       |                                  |
| 88        | N            | O10         | 37                        | 0.185%                      | 0       |                                  |
| 88        | N            | O11         | 54                        | 0.270%                      | 0       |                                  |
| 88        | N            | O12         | 229                       | 1.145%                      | 0       |                                  |
| 88        | N            | O13         | 2                         | 0.010%                      | 0       |                                  |
| 88        | O            | O11         | 341                       | 1.705%                      | 0       |                                  |
| 88        | O            | O12         | 374                       | 1.870%                      | 0       |                                  |
| 89        | N            | O11         | 11                        | 0.055%                      | 0       |                                  |
| 89        | N            | O12         | 1                         | 0.005%                      | 0       |                                  |
| 89        | O            | O7          | 11                        | 0.055%                      | 0       |                                  |
| 89        | O            | O11         | 8                         | 0.040%                      | 0       |                                  |
Hydrogen bonds observed during last 400ns of MD simulations between hFKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-Score | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 89        | O            | O12         | 195                       | 0.975%                        | 0       |                                   |
| 90        | N            | O3          | 1                         | 0.005%                        | 0       |                                   |
| 90        | N            | O11         | 64                        | 0.320%                        | 0       |                                   |
| 90        | N            | O12         | 95                        | 0.475%                        | 0       |                                   |
| 90        | O            | O6          | 2                         | 0.010%                        | 0       |                                   |
| 90        | O            | O7          | 20                        | 0.100%                        | 0       |                                   |
| 90        | O            | O12         | 7                         | 0.035%                        | 0       |                                   |
| 91        | N            | O7          | 77                        | 0.385%                        | 0       |                                   |
| 91        | N            | O8          | 3                         | 0.015%                        | 0       |                                   |
| 91        | N            | O11         | 3                         | 0.015%                        | 0       |                                   |
| 91        | N            | O12         | 9                         | 0.045%                        | 0       |                                   |
| 91        | O            | O6          | 32                        | 0.160%                        | 0       | 0.885%                            |
| 91        | O            | O7          | 39                        | 0.195%                        | 0       |                                   |
| 91        | O            | O8          | 5                         | 0.025%                        | 0       |                                   |
| 91        | O            | O12         | 9                         | 0.045%                        | 0       |                                   |
Hydrogen bonds observed during last 400ns of MD simulations between *AfFKBP12* and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 27        | OH           | O4         | 110                       | 0.458%                        | 0       | 3.453%                            |
| 27        | OH           | O5         | 712                       | 2.966%                        | 0       |                                   |
| 27        | OH           | O6         | 7                         | 0.029%                        | 0       |                                   |
| 28        | O            | O4         | 2                         | 0.008%                        | 0       | 0.008%                            |
| 37        | O            | O6         | 34                        | 0.142%                        | 0       | 0.142%                            |
| 38        | N            | O4         | 210                       | 0.875%                        | 0       |                                   |
| 38        | N            | O6         | 5138                      | 21.403%                       | 3       |                                   |
| 38        | OD1          | O4         | 29                        | 0.121%                        | 0       |                                   |
| 38        | OD1          | O5         | 49                        | 0.204%                        | 0       |                                   |
| 38        | OD1          | O6         | 933                       | 3.887%                        | 0       |                                   |
| 38        | OD1          | O7         | 1                         | 0.004%                        | 0       |                                   |
| 38        | OD2          | O4         | 33                        | 0.137%                        | 0       | 47.347%                           |
| 38        | OD2          | O5         | 53                        | 0.221%                        | 0       |                                   |
| 38        | OD2          | O6         | 828                       | 3.449%                        | 0       |                                   |
| 38        | O            | O4         | 1400                      | 5.832%                        | 1       |                                   |
| 38        | O            | O5         | 317                       | 1.321%                        | 0       |                                   |
| 38        | O            | O6         | 2373                      | 9.885%                        | 1       |                                   |
| 43        | NE           | O7         | 2                         | 0.008%                        | 0       |                                   |
| 43        | NH1          | O4         | 267                       | 1.112%                        | 0       |                                   |
| 43        | NH1          | O5         | 102                       | 0.425%                        | 0       |                                   |
| 43        | NH1          | O6         | 4                         | 0.017%                        | 0       |                                   |
| 43        | NH1          | O7         | 25                        | 0.104%                        | 0       |                                   |
| 43        | NH1          | O8         | 13                        | 0.054%                        | 0       | 2.391%                            |
| 43        | NH2          | O4         | 13                        | 0.054%                        | 0       |                                   |
| 43        | NH2          | O5         | 9                         | 0.037%                        | 0       |                                   |
| 43        | NH2          | O6         | 110                       | 0.458%                        | 0       |                                   |
| 43        | NH2          | O7         | 22                        | 0.092%                        | 0       |                                   |
| 43        | NH2          | O8         | 7                         | 0.029%                        | 0       |                                   |
| 49        | OG1          | O2         | 3                         | 0.012%                        | 0       | 0.012%                            |
| 54        | N            | O11        | 43                        | 0.179%                        | 0       |                                   |
| 54        | O            | O10        | 17                        | 0.071%                        | 0       | 2.970%                            |
| 54        | O            | O11        | 54                        | 0.225%                        | 0       |                                   |
| 55        | NE           | O10        | 25                        | 0.104%                        | 0       |                                   |
| 55        | NE           | O11        | 24                        | 0.100%                        | 0       |                                   |
| 55        | NE           | O12        | 35                        | 0.146%                        | 0       |                                   |
| 55        | NH1          | O10        | 68                        | 0.283%                        | 0       |                                   |
| 55        | NH1          | O11        | 91                        | 0.379%                        | 0       |                                   |
| 55        | NH1          | O12        | 93                        | 0.387%                        | 0       |                                   |
| 55        | NH1          | O9         | 2                         | 0.008%                        | 0       |                                   |
| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|----------------------------------|
| 55        | NH2          | O10         | 15                        | 0.062%                        | 0       | 34.866%                          |
| 55        | NH2          | O11         | 30                        | 0.125%                        | 0       |                                  |
| 55        | NH2          | O12         | 36                        | 0.150%                        | 0       |                                  |
| 55        | NH2          | O9          | 3                         | 0.012%                        | 0       |                                  |
| 55        | O            | O10         | 7787                      | 32.438%                       | 4       |                                  |
| 55        | O            | O11         | 78                        | 0.325%                        | 0       |                                  |
| 55        | O            | O12         | 64                        | 0.267%                        | 0       |                                  |
| 56        | N            | O10         | 5                         | 0.021%                        | 0       |                                  |
| 56        | N            | O11         | 1                         | 0.004%                        | 0       | 0.062%                           |
| 56        | O            | O11         | 6                         | 0.025%                        | 0       |                                  |
| 56        | O            | O12         | 3                         | 0.012%                        | 0       |                                  |
| 57        | N            | O2          | 17050                     | 71.024%                       | 10      | 71.024%                          |
| 58        | NZ           | O11         | 2                         | 0.008%                        | 0       | 0.008%                           |
| 60        | NE1          | O3          | 1733                      | 7.219%                        | 1       | 7.244%                           |
| 60        | NE1          | O4          | 6                         | 0.025%                        | 0       |                                  |
| 82        | O            | O11         | 8                         | 0.033%                        | 0       | 0.100%                           |
| 82        | O            | O12         | 16                        | 0.067%                        | 0       |                                  |
| 83        | OH           | O1          | 24                        | 0.100%                        | 0       |                                  |
| 83        | OH           | O11         | 20                        | 0.083%                        | 0       |                                  |
| 83        | OH           | O12         | 95                        | 0.396%                        | 0       |                                  |
| 83        | OH           | O2          | 13                        | 0.054%                        | 0       | 5.345%                           |
| 83        | OH           | O3          | 883                       | 3.678%                        | 0       |                                  |
| 83        | OH           | O6          | 17                        | 0.071%                        | 0       |                                  |
| 83        | O            | O11         | 30                        | 0.125%                        | 0       |                                  |
| 83        | O            | O12         | 201                       | 0.837%                        | 0       |                                  |
| 84        | N            | O11         | 947                       | 3.945%                        | 0       |                                  |
| 84        | N            | O12         | 149                       | 0.621%                        | 0       | 5.361%                           |
| 84        | O            | O11         | 100                       | 0.417%                        | 0       |                                  |
| 84        | O            | O12         | 91                        | 0.379%                        | 0       |                                  |
| 85        | N            | O11         | 458                       | 1.908%                        | 0       |                                  |
| 85        | N            | O12         | 501                       | 2.087%                        | 0       |                                  |
| 85        | O            | O10         | 9                         | 0.037%                        | 0       | 8.319%                           |
| 85        | O            | O11         | 140                       | 0.583%                        | 0       |                                  |
| 85        | O            | O12         | 889                       | 3.703%                        | 0       |                                  |
| 86        | NE           | O11         | 138                       | 0.575%                        | 0       |                                  |
| 86        | NE           | O12         | 73                        | 0.304%                        | 0       |                                  |
| 86        | NE           | O7          | 67                        | 0.279%                        | 0       |                                  |
| 86        | NH1          | O11         | 114                       | 0.475%                        | 0       |                                  |
| 86        | NH1          | O12         | 117                       | 0.487%                        | 0       |                                  |
| 86        | NH1          | O6          | 5                         | 0.021%                        | 0       |                                  |
Hydrogen bonds observed during last 400ns of MD simulations between AfFKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|----------------------------|--------------------------------|---------|-----------------------------------|
| 86        | NH1          | O7         | 46                         | 0.192%                         | 0       | 10.027%                           |
| 86        | NH1          | O8         | 2                          | 0.008%                         | 0       |                                   |
| 86        | NH1          | O9         | 2                          | 0.008%                         | 0       |                                   |
| 86        | NH2          | O10        | 1                          | 0.004%                         | 0       |                                   |
| 86        | NH2          | O11        | 115                        | 0.479%                         | 0       |                                   |
| 86        | NH2          | O12        | 34                         | 0.142%                         | 0       |                                   |
| 86        | NH2          | O6         | 11                         | 0.046%                         | 0       |                                   |
| 86        | NH2          | O7         | 34                         | 0.142%                         | 0       |                                   |
| 86        | N            | O11        | 60                         | 0.250%                         | 0       |                                   |
| 86        | N            | O12        | 158                        | 0.658%                         | 0       |                                   |
| 86        | O            | O10        | 91                         | 0.379%                         | 0       |                                   |
| 86        | O            | O11        | 58                         | 0.242%                         | 0       |                                   |
| 86        | O            | O12        | 1274                       | 5.307%                         | 1       |                                   |
| 86        | O            | O7         | 6                          | 0.025%                         | 0       |                                   |
| 87        | N            | O11        | 79                         | 0.329%                         | 0       |                                   |
| 87        | N            | O12        | 250                        | 1.041%                         | 0       |                                   |
| 87        | N            | O7         | 1                          | 0.004%                         | 0       | 3.695%                            |
| 87        | O            | O11        | 41                         | 0.171%                         | 0       |                                   |
| 87        | O            | O12        | 516                        | 2.149%                         | 0       |                                   |
| 88        | N            | O11        | 283                        | 1.179%                         | 0       |                                   |
| 88        | N            | O12        | 106                        | 0.442%                         | 0       |                                   |
| 88        | N            | O9         | 150                        | 0.625%                         | 0       |                                   |
| 88        | O            | O10        | 156                        | 0.650%                         | 0       | 7.082%                            |
| 88        | O            | O11        | 121                        | 0.504%                         | 0       |                                   |
| 88        | O            | O12        | 877                        | 3.653%                         | 0       |                                   |
| 88        | O            | O9         | 7                          | 0.029%                         | 0       |                                   |
| 89        | N            | O12        | 4                          | 0.017%                         | 0       |                                   |
| 89        | N            | O9         | 3                          | 0.012%                         | 0       |                                   |
| 89        | O            | O10        | 70                         | 0.292%                         | 0       |                                   |
| 89        | O            | O11        | 66                         | 0.275%                         | 0       | 1.616%                            |
| 89        | O            | O12        | 75                         | 0.312%                         | 0       |                                   |
| 89        | O            | O6         | 11                         | 0.046%                         | 0       |                                   |
| 89        | O            | O7         | 13                         | 0.054%                         | 0       |                                   |
| 89        | O            | O9         | 146                        | 0.608%                         | 0       |                                   |
| 90        | N            | O11        | 93                         | 0.387%                         | 0       |                                   |
| 90        | N            | O12        | 14                         | 0.058%                         | 0       |                                   |
| 90        | N            | O6         | 1                          | 0.004%                         | 0       |                                   |
| 90        | N            | O7         | 1                          | 0.004%                         | 0       |                                   |
| 90        | N            | O9         | 12                         | 0.050%                         | 0       |                                   |
| 90        | O            | O11        | 18                         | 0.075%                         | 0       | 0.683%                            |
Hydrogen bonds observed during last 400ns of MD simulations between AfFKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond’s existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|--------------------------------|---------|-------------------------------------|
| 90        | O            | O12        | 10                        | 0.042%                         | 0       |                                     |
| 90        | O            | O3         | 1                         | 0.004%                         | 0       |                                     |
| 90        | O            | O6         | 12                        | 0.050%                         | 0       |                                     |
| 90        | O            | O7         | 1                         | 0.004%                         | 0       |                                     |
| 90        | O            | O9         | 1                         | 0.004%                         | 0       |                                     |
| 91        | N            | O11        | 41                        | 0.171%                         | 0       |                                     |
| 91        | N            | O3         | 4                         | 0.017%                         | 0       |                                     |
| 91        | N            | O6         | 3                         | 0.012%                         | 0       |                                     |
| 91        | N            | O7         | 49                        | 0.204%                         | 0       |                                     |
| 91        | N            | O9         | 67                        | 0.279%                         | 0       | 0.921%                              |
| 91        | O            | O11        | 2                         | 0.008%                         | 0       |                                     |
| 91        | O            | O12        | 2                         | 0.008%                         | 0       |                                     |
| 91        | O            | O6         | 51                        | 0.212%                         | 0       |                                     |
| 91        | O            | O7         | 2                         | 0.008%                         | 0       |                                     |
| 92        | N            | O11        | 4                         | 0.017%                         | 0       |                                     |
| 92        | N            | O6         | 1                         | 0.004%                         | 0       | 0.025%                              |
| 92        | O            | O11        | 1                         | 0.004%                         | 0       |                                     |
Hydrogen bonds observed during last 400ns of MD simulations between *Af*FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond’s existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|--------------------------|--------------------------------|---------|------------------------------------|
| 27        | OH O4        | 95          | 0.475%                   | 0                              |         |                                    |
| 27        | OH O5        | 6           | 0.030%                   | 0                              |         |                                    |
| 27        | OH O6        | 1987        | 9.933%                   | 2                              |         | 13.837%                            |
| 27        | OH O8        | 679         | 3.394%                   | 0                              |         |                                    |
| 27        | O O4         | 1           | 0.005%                   | 0                              |         |                                    |
| 37        | O O4         | 1           | 0.005%                   | 0                              |         | 0.005%                             |
| 38        | N O4         | 1           | 0.005%                   | 0                              |         |                                    |
| 38        | N O6         | 18          | 0.090%                   | 0                              |         |                                    |
| 38        | OD1 O4       | 189         | 0.945%                   | 0                              |         |                                    |
| 38        | OD1 O6       | 6167        | 30.827%                  | 6                              |         |                                    |
| 38        | OD1 O7       | 1           | 0.005%                   | 0                              |         |                                    |
| 38        | OD2 O4       | 172         | 0.860%                   | 0                              |         |                                    |
| 38        | OD2 O6       | 5759        | 28.788%                  | 6                              |         | 72.287%                            |
| 38        | OD2 O7       | 2           | 0.010%                   | 0                              |         |                                    |
| 38        | O O4         | 34          | 0.170%                   | 0                              |         |                                    |
| 38        | O O6         | 2115        | 10.572%                  | 2                              |         |                                    |
| 38        | O O8         | 3           | 0.015%                   | 0                              |         |                                    |
| 39        | N O6         | 6           | 0.030%                   | 0                              |         |                                    |
| 39        | OG O6        | 2           | 0.010%                   | 0                              |         |                                    |
| 39        | OG O7        | 1           | 0.005%                   | 0                              |         |                                    |
| 39        | OG O8        | 4           | 0.020%                   | 0                              |         | 0.210%                             |
| 39        | O O6         | 26          | 0.130%                   | 0                              |         |                                    |
| 39        | O O8         | 3           | 0.015%                   | 0                              |         |                                    |
| 40        | OG O4        | 3           | 0.015%                   | 0                              |         |                                    |
| 40        | OG O6        | 9           | 0.045%                   | 0                              |         | 0.060%                             |
| 43        | NE O6        | 9           | 0.045%                   | 0                              |         |                                    |
| 43        | NE O8        | 3           | 0.015%                   | 0                              |         |                                    |
| 43        | NH1 O5       | 5           | 0.025%                   | 0                              |         |                                    |
| 43        | NH1 O6       | 50          | 0.250%                   | 0                              |         |                                    |
| 43        | NH1 O8       | 67          | 0.335%                   | 0                              |         |                                    |
| 43        | NH1 O13      | 6           | 0.030%                   | 0                              |         | 1.795%                             |
| 43        | NH2 O5       | 5           | 0.025%                   | 0                              |         |                                    |
| 43        | NH2 O6       | 138         | 0.690%                   | 0                              |         |                                    |
| 43        | NH2 O7       | 3           | 0.015%                   | 0                              |         |                                    |
| 43        | NH2 O8       | 66          | 0.330%                   | 0                              |         |                                    |
| 43        | NH2 O13      | 7           | 0.035%                   | 0                              |         |                                    |
| 48        | O N54        | 1           | 0.005%                   | 0                              |         |                                    |
| 48        | O N55        | 12          | 0.060%                   | 0                              |         |                                    |
| 48        | O O10        | 1           | 0.005%                   | 0                              |         | 0.260%                             |
| 48        | O O12        | 6           | 0.030%                   | 0                              |         |                                    |
Hydrogen bonds observed during last 400ns of MD simulations between Af FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|--------------------------------|---------|-----------------------------------|
| 48        | O            | O13         | 32                        | 0.160%                         | 0       |                                   |
| 49        | OG1          | N54         | 6                         | 0.030%                         | 0       |                                   |
| 49        | OG1          | N55         | 194                       | 0.970%                         | 0       |                                   |
| 49        | OG1          | O2          | 5                         | 0.025%                         | 0       | 2.129%                            |
| 49        | OG1          | O10         | 172                       | 0.860%                         | 0       |                                   |
| 49        | OG1          | O13         | 49                        | 0.245%                         | 0       |                                   |
| 50        | NE2          | N55         | 1                         | 0.05%                          | 0       | 4.369%                            |
| 50        | NE2          | O10         | 14                        | 0.07%                          | 0       |                                   |
| 50        | NE2          | O13         | 10                        | 0.05%                          | 0       |                                   |
| 50        | N            | O10         | 47                        | 0.235%                         | 0       |                                   |
| 50        | N            | O12         | 12                        | 0.06%                          | 0       |                                   |
| 50        | N            | O13         | 723                       | 3.614%                         | 0       |                                   |
| 50        | OE1          | N55         | 47                        | 0.235%                         | 0       |                                   |
| 50        | OE1          | O10         | 13                        | 0.065%                         | 0       |                                   |
| 50        | OE1          | O13         | 3                         | 0.015%                         | 0       |                                   |
| 50        | O            | O10         | 4                         | 0.02%                          | 0       |                                   |
| 54        | O            | O10         | 45                        | 0.225%                         | 0       | 0.975%                            |
| 54        | O            | O11         | 46                        | 0.230%                         | 0       |                                   |
| 54        | O            | O12         | 104                       | 0.520%                         | 0       |                                   |
| 55        | NE           | N54         | 1                         | 0.05%                          | 0       |                                   |
| 55        | NE           | N55         | 1                         | 0.05%                          | 0       |                                   |
| 55        | NE           | O10         | 11                        | 0.055%                         | 0       |                                   |
| 55        | NE           | O11         | 14                        | 0.07%                          | 0       |                                   |
| 55        | NE           | O12         | 2                         | 0.01%                          | 0       |                                   |
| 55        | NE           | O13         | 44                        | 0.22%                          | 0       |                                   |
| 55        | NH1          | N54         | 4                         | 0.02%                          | 0       |                                   |
| 55        | NH1          | N55         | 2                         | 0.01%                          | 0       |                                   |
| 55        | NH1          | O10         | 5                         | 0.025%                         | 0       |                                   |
| 55        | NH1          | O11         | 12                        | 0.06%                          | 0       |                                   |
| 55        | NH1          | O12         | 23                        | 0.115%                         | 0       |                                   |
| 55        | NH1          | O13         | 149                       | 0.745%                         | 0       | 30.647%                           |
| 55        | NH2          | N54         | 1                         | 0.05%                          | 0       |                                   |
| 55        | NH2          | N55         | 1                         | 0.05%                          | 0       |                                   |
| 55        | NH2          | O10         | 2                         | 0.01%                          | 0       |                                   |
| 55        | NH2          | O11         | 5                         | 0.025%                         | 0       |                                   |
| 55        | NH2          | O12         | 18                        | 0.09%                          | 0       |                                   |
| 55        | NH2          | O13         | 61                        | 0.305%                         | 0       |                                   |
| 55        | N            | O10         | 22                        | 0.11%                          | 0       |                                   |
| 55        | O            | N55         | 209                       | 1.045%                         | 0       |                                   |
| 55        | O            | O10         | 5513                      | 27.558%                        | 5       |                                   |
Hydrogen bonds observed during last 400ns of MD simulations between *AfFKBP12* and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|--------------------------------|---------|-----------------------------------|
| 55        | O            | O11         | 24                        | 0.120%                         | 0       | 0                                 |
| 55        | O            | O12         | 7                         | 0.035%                         | 0       | 0                                 |
| 56        | N            | O10         | 128                       | 0.640%                         | 0       | 0.685%                            |
| 56        | O            | O11         | 9                         | 0.045%                         | 0       |                                    |
| 57        | N            | O2          | 5508                      | 27.533%                        | 5       | 27.563%                           |
| 57        | N            | O10         | 6                         | 0.030%                         | 0       |                                    |
| 60        | NE1          | O2          | 1                         | 0.005%                         | 0       |                                    |
| 60        | NE1          | O3          | 921                       | 4.604%                         | 1       | 4.754%                            |
| 60        | NE1          | O4          | 29                        | 0.145%                         | 0       |                                    |
| 82        | O            | O11         | 1                         | 0.005%                         | 0       | 0.020%                            |
| 82        | O            | O12         | 3                         | 0.015%                         | 0       |                                    |
| 83        | OH           | N55         | 7                         | 0.035%                         | 0       |                                    |
| 83        | OH           | O2          | 7                         | 0.035%                         | 0       |                                    |
| 83        | OH           | O3          | 343                       | 1.715%                         | 0       |                                    |
| 83        | OH           | O7          | 21                        | 0.105%                         | 0       |                                    |
| 83        | OH           | O10         | 22                        | 0.110%                         | 0       |                                    |
| 83        | OH           | O11         | 99                        | 0.495%                         | 0       |                                    |
| 83        | OH           | O12         | 105                       | 0.525%                         | 0       |                                    |
| 83        | OH           | O13         | 3                         | 0.015%                         | 0       |                                    |
| 83        | O            | O11         | 2                         | 0.010%                         | 0       |                                    |
| 83        | O            | O12         | 3                         | 0.015%                         | 0       |                                    |
| 84        | N            | O11         | 2                         | 0.010%                         | 0       |                                    |
| 84        | N            | O12         | 4                         | 0.020%                         | 0       | 0.130%                            |
| 84        | O            | O12         | 20                        | 0.100%                         | 0       |                                    |
| 85        | N            | O12         | 1                         | 0.005%                         | 0       |                                    |
| 85        | O            | O11         | 12                        | 0.060%                         | 0       | 0.835%                            |
| 85        | O            | O12         | 154                       | 0.770%                         | 0       |                                    |
| 86        | NE           | O10         | 3                         | 0.015%                         | 0       |                                    |
| 86        | NE           | O11         | 79                        | 0.395%                         | 0       |                                    |
| 86        | NE           | O12         | 226                       | 1.130%                         | 0       |                                    |
| 86        | NH1          | O7           | 1                         | 0.005%                         | 0       |                                    |
| 86        | NH1          | O10          | 12                        | 0.060%                         | 0       |                                    |
| 86        | NH1          | O11          | 216                       | 1.080%                         | 0       |                                    |
| 86        | NH1          | O12          | 726                       | 3.629%                         | 0       |                                    |
| 86        | NH2          | O10          | 2                         | 0.010%                         | 0       | 8.358%                            |
| 86        | NH2          | O11          | 125                       | 0.625%                         | 0       |                                    |
| 86        | NH2          | O12          | 236                       | 1.180%                         | 0       |                                    |
| 86        | N            | O12          | 3                         | 0.015%                         | 0       |                                    |
| 86        | O            | O2           | 2                         | 0.010%                         | 0       |                                    |
| 86        | O            | O7           | 2                         | 0.010%                         | 0       |                                    |
Hydrogen bonds observed during last 400ns of MD simulations between *Af*FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------------------------------------------|
| 86        | O            | O11         | 10                        | 0.050%                        | 0                                           |
| 86        | O            | O12         | 29                        | 0.145%                        | 0                                           |
| 87        | N            | O11         | 148                       | 0.740%                        | 0                                           |
| 87        | N            | O12         | 276                       | 1.380%                        | 0                                           |
| 87        | O            | O11         | 154                       | 0.770%                        | 0                                           |
| 87        | O            | O12         | 249                       | 1.245%                        | 0                                           |
| 88        | N            | O3          | 10                        | 0.050%                        | 0                                           |
| 88        | N            | O12         | 1                         | 0.005%                        | 0.055%                                      |
| 89        | N            | O12         | 1                         | 0.005%                        | 0                                           |
| 89        | O            | O3          | 8                         | 0.040%                        | 0                                           |
| 89        | O            | O6          | 66                        | 0.330%                        | 0                                           |
| 89        | O            | O7          | 26                        | 0.130%                        | 0.550%                                      |
| 89        | O            | O8          | 6                         | 0.030%                        | 0                                           |
| 89        | O            | O11         | 2                         | 0.010%                        | 0                                           |
| 89        | O            | O12         | 1                         | 0.005%                        | 0                                           |
| 90        | O            | O11         | 1                         | 0.005%                        | 0.005%                                      |
| 91        | O            | O3          | 8                         | 0.040%                        | 0.040%                                      |
| 92        | N            | O3          | 1                         | 0.005%                        | 0.005%                                      |
| 111       | NH1          | O13         | 3                         | 0.015%                        | 0                                           |
| 111       | NH2          | O13         | 6                         | 0.030%                        | 0.045%                                      |
## Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|-------------------------------|---------|------------------------------------|
| 27        | OH           | O4         | 8                         | 0.040%                        | 0       | 1.590%                             |
| 27        | OH           | O5         | 277                       | 1.385%                        | 0       |                                    |
| 27        | OH           | O6         | 33                        | 0.165%                        | 0       |                                    |
| 29        | N            | O4         | 1                         | 0.005%                        | 0       | 0.020%                             |
| 29        | N            | O6         | 3                         | 0.015%                        | 0       |                                    |
| 37        | O            | O6         | 20                        | 0.100%                        | 0       | 0.100%                             |
| 38        | N            | O4         | 2                         | 0.010%                        | 0       |                                    |
| 38        | N            | O6         | 155                       | 0.775%                        | 0       |                                    |
| 38        | N            | O7         | 23                        | 0.115%                        | 0       |                                    |
| 38        | OD1          | O4         | 17                        | 0.085%                        | 0       |                                    |
| 38        | OD1          | O5         | 175                       | 0.875%                        | 0       |                                    |
| 38        | OD1          | O6         | 371                       | 1.855%                        | 0       |                                    |
| 38        | OD1          | O7         | 1                         | 0.005%                        | 0       | 8.953%                             |
| 38        | OD2          | O4         | 14                        | 0.070%                        | 0       |                                    |
| 38        | OD2          | O5         | 203                       | 1.015%                        | 0       |                                    |
| 38        | OD2          | O6         | 342                       | 1.710%                        | 0       |                                    |
| 38        | OD2          | O7         | 1                         | 0.005%                        | 0       |                                    |
| 38        | O            | O4         | 48                        | 0.240%                        | 0       |                                    |
| 38        | O            | O5         | 10                        | 0.050%                        | 0       |                                    |
| 38        | O            | O6         | 429                       | 2.144%                        | 0       |                                    |
| 39        | OG           | O6         | 4                         | 0.020%                        | 0       | 0.020%                             |
| 43        | NE           | O6         | 7                         | 0.035%                        | 0       |                                    |
| 43        | NH1          | O7         | 30                        | 0.150%                        | 0       |                                    |
| 43        | NH1          | O8         | 8                         | 0.040%                        | 0       | 1.355%                             |
| 43        | NH2          | O6         | 4                         | 0.020%                        | 0       |                                    |
| 43        | NH2          | O7         | 160                       | 0.800%                        | 0       |                                    |
| 43        | NH2          | O8         | 62                        | 0.310%                        | 0       |                                    |
| 50        | OG1          | O10        | 6                         | 0.030%                        | 0       | 0.035%                             |
| 53        | O            | O10        | 4                         | 0.020%                        | 0       | 0.020%                             |
| 54        | N            | O11        | 3                         | 0.015%                        | 0       |                                    |
| 54        | O            | O11        | 5                         | 0.025%                        | 0       | 0.440%                             |
| 54        | O            | O12        | 80                        | 0.400%                        | 0       |                                    |
| 55        | NE2          | O10        | 196                       | 0.980%                        | 0       |                                    |
| 55        | NE2          | O11        | 48                        | 0.240%                        | 0       |                                    |
| 55        | NE2          | O12        | 32                        | 0.160%                        | 0       |                                    |
| 55        | NE2          | O2         | 1                         | 0.005%                        | 0       |                                    |
| 55        | N            | O10        | 25                        | 0.125%                        | 0       |                                    |
| 55        | OE1          | O10        | 315                       | 1.575%                        | 0       |                                    |
## Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|---------------------------|------------------------------|---------|-------------------------------------|
| 55        | OE1          | O11        | 7                         | 0.035%                       | 0       | 35.276%                             |
| 55        | OE1          | O12        | 133                       | 0.665%                       | 0       |                                     |
| 55        | O            | O9         | 2                         | 0.010%                       | 0       |                                     |
| 55        | O            | O1          | 1                         | 0.005%                       | 0       |                                     |
| 55        | O            | O10        | 5978                      | 29.883%                      | 4       |                                     |
| 55        | O            | O11        | 6                         | 0.030%                       | 0       |                                     |
| 55        | O            | O12        | 2                         | 0.010%                       | 0       |                                     |
| 55        | O            | O2         | 311                       | 1.555%                       | 0       |                                     |
| 56        | N            | O10        | 15                        | 0.075%                       | 0       |                                     |
| 56        | O            | O11        | 7                         | 0.035%                       | 0       | 0.120%                              |
| 56        | O            | O12        | 2                         | 0.010%                       | 0       |                                     |
| 57        | N            | O2         | 13379                     | 66.878%                      | 10      | 66.893%                             |
| 57        | N            | O3         | 3                         | 0.015%                       | 0       |                                     |
| 58        | NZ           | O11        | 2                         | 0.010%                       | 0       | 0.010%                              |
| 60        | NE1          | O3         | 3049                      | 15.241%                      | 2       | 15.491%                             |
| 60        | NE1          | O4         | 50                        | 0.250%                       | 0       |                                     |
| 82        | O            | O11        | 1                         | 0.005%                       | 0       |                                     |
| 82        | O            | O12        | 4                         | 0.020%                       | 0       | 0.040%                              |
| 82        | O            | O3         | 3                         | 0.015%                       | 0       |                                     |
| 83        | OH           | O11        | 216                       | 1.080%                       | 0       |                                     |
| 83        | OH           | O12        | 307                       | 1.535%                       | 0       |                                     |
| 83        | OH           | O3         | 11                        | 0.055%                       | 0       | 2.914%                              |
| 83        | OH           | O9         | 18                        | 0.090%                       | 0       |                                     |
| 83        | O            | O11        | 7                         | 0.035%                       | 0       |                                     |
| 83        | O            | O12        | 24                        | 0.120%                       | 0       |                                     |
| 84        | N            | O11        | 696                       | 3.479%                       | 0       |                                     |
| 84        | N            | O12        | 159                       | 0.795%                       | 0       | 5.224%                              |
| 84        | O            | O11        | 98                        | 0.490%                       | 0       |                                     |
| 84        | O            | O12        | 92                        | 0.460%                       | 0       |                                     |
| 85        | N            | O11        | 603                       | 3.014%                       | 0       |                                     |
| 85        | N            | O12        | 146                       | 0.730%                       | 0       |                                     |
| 85        | OE1          | O12        | 46                        | 0.230%                       | 0       | 6.573%                              |
| 85        | OE2          | O12        | 30                        | 0.150%                       | 0       |                                     |
| 85        | O            | O11        | 41                        | 0.205%                       | 0       |                                     |
| 85        | O            | O12        | 449                       | 2.244%                       | 0       |                                     |
| 86        | NE           | O11        | 187                       | 0.935%                       | 0       |                                     |
| 86        | NE           | O12        | 126                       | 0.630%                       | 0       |                                     |
| 86        | NH1          | O10        | 2                         | 0.010%                       | 0       |                                     |
| 86        | NH1          | O11        | 334                       | 1.670%                       | 0       |                                     |
Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and FK506

| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|------------|----------------------------|-------------------------------|---------|-----------------------------------|
| 86        | NH1          | O12        | 277                        | 1.385%                        | 0       | 14.806%                           |
| 86        | NH2          | O10        | 3                          | 0.015%                        | 0       |                                   |
| 86        | NH2          | O11        | 132                        | 0.660%                        | 0       |                                   |
| 86        | NH2          | O12        | 72                         | 0.360%                        | 0       |                                   |
| 86        | N            | O11        | 489                        | 2.444%                        | 0       |                                   |
| 86        | N            | O12        | 891                        | 4.454%                        | 0       |                                   |
| 86        | O            | O10        | 4                          | 0.020%                        | 0       |                                   |
| 86        | O            | O11        | 67                         | 0.335%                        | 0       |                                   |
| 86        | O            | O12        | 378                        | 1.890%                        | 0       |                                   |
| 87        | N            | O11        | 117                        | 0.585%                        | 0       | 4.189%                            |
| 87        | N            | O12        | 242                        | 1.210%                        | 0       |                                   |
| 87        | O            | O11        | 164                        | 0.820%                        | 0       |                                   |
| 87        | O            | O12        | 315                        | 1.575%                        | 0       |                                   |
| 88        | N            | O10        | 4                          | 0.020%                        | 0       |                                   |
| 88        | N            | O11        | 170                        | 0.850%                        | 0       |                                   |
| 88        | N            | O12        | 372                        | 1.860%                        | 0       |                                   |
| 88        | N            | O9         | 5                          | 0.025%                        | 0       |                                   |
| 88        | OH           | O10        | 2                          | 0.010%                        | 0       |                                   |
| 88        | OH           | O11        | 1                          | 0.005%                        | 0       |                                   |
| 88        | OH           | O12        | 40                         | 0.200%                        | 0       | 6.338%                            |
| 88        | OH           | O3         | 39                         | 0.195%                        | 0       |                                   |
| 88        | OH           | O6         | 1                          | 0.005%                        | 0       |                                   |
| 88        | OH           | O7         | 12                         | 0.060%                        | 0       |                                   |
| 88        | OH           | O9         | 5                          | 0.025%                        | 0       |                                   |
| 88        | O            | O11        | 108                        | 0.540%                        | 0       |                                   |
| 88        | O            | O12        | 509                        | 2.544%                        | 0       |                                   |
| 89        | N            | O11        | 1                          | 0.005%                        | 0       |                                   |
| 89        | N            | O12        | 1                          | 0.005%                        | 0       |                                   |
| 89        | O            | O11        | 5                          | 0.025%                        | 0       | 0.320%                            |
| 89        | O            | O12        | 51                         | 0.255%                        | 0       |                                   |
| 89        | O            | O6         | 4                          | 0.020%                        | 0       |                                   |
| 89        | O            | O7         | 2                          | 0.010%                        | 0       |                                   |
| 90        | N            | O11        | 56                         | 0.280%                        | 0       | 0.710%                            |
| 90        | N            | O12        | 21                         | 0.105%                        | 0       |                                   |
| 90        | N            | O7         | 2                          | 0.010%                        | 0       |                                   |
| 90        | O            | O11        | 12                         | 0.060%                        | 0       |                                   |
| 90        | O            | O12        | 9                          | 0.045%                        | 0       |                                   |
| 90        | O            | O6         | 38                         | 0.190%                        | 0       |                                   |
| 90        | O            | O7         | 4                          | 0.020%                        | 0       |                                   |
| 91        | N            | O11        | 6                          | 0.030%                        | 0       |                                   |
| Residue # | residue atom | FK506 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|--------------------------------|---------|-------------------------------------|
| 91        | N            | O12         | 1                         | 0.005%                         | 0       |                                     |
| 91        | N            | O6          | 18                        | 0.090%                         | 0       |                                     |
| 91        | N            | O7          | 8                         | 0.040%                         | 0       | 0.220%                              |
| 91        | O            | O12         | 1                         | 0.005%                         | 0       |                                     |
| 91        | O            | O6          | 3                         | 0.015%                         | 0       |                                     |
| 91        | O            | O7          | 7                         | 0.035%                         | 0       |                                     |
| 92        | N            | O4          | 2                         | 0.010%                         | 0       | 0.050%                              |
| 92        | N            | O6          | 8                         | 0.040%                         | 0       |                                     |
| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|------------------------------|---------|----------------------------------|
| 22        | NZ           | O13         | 15                        | 0.075%                       | 0       | 0.075%                           |
| 27        | OH           | O4          | 15                        | 0.075%                       | 0       |                                  |
| 27        | OH           | O5          | 12                        | 0.060%                       | 0       |                                  |
| 27        | OH           | O6          | 1312                      | 6.558%                       | 1       | 14.691%                          |
| 27        | OH           | O8          | 1599                      | 7.993%                       | 1       |                                  |
| 27        | OH           | O13         | 1                         | 0.005%                       | 0       |                                  |
| 37        | O            | O4          | 1                         | 0.005%                       | 0       |                                  |
| 37        | O            | O6          | 32                        | 0.160%                       | 0       | 0.165%                           |
| 38        | N            | O4          | 5                         | 0.025%                       | 0       |                                  |
| 38        | N            | O6          | 109                       | 0.545%                       | 0       |                                  |
| 38        | N            | O8          | 4                         | 0.020%                       | 0       |                                  |
| 38        | OD1          | O4          | 329                       | 1.645%                       | 0       |                                  |
| 38        | OD1          | O5          | 1                         | 0.005%                       | 0       |                                  |
| 38        | OD1          | O6          | 5650                      | 28.243%                      | 6       |                                  |
| 38        | OD1          | O7          | 6                         | 0.030%                       | 0       |                                  |
| 38        | OD1          | O8          | 21                        | 0.105%                       | 0       |                                  |
| 38        | OD2          | O4          | 360                       | 1.800%                       | 0       | 68.008%                          |
| 38        | OD2          | O5          | 3                         | 0.015%                       | 0       |                                  |
| 38        | OD2          | O6          | 6057                      | 30.277%                      | 6       |                                  |
| 38        | OD2          | O7          | 4                         | 0.020%                       | 0       |                                  |
| 38        | OD2          | O8          | 24                        | 0.120%                       | 0       |                                  |
| 38        | O            | O4          | 11                        | 0.055%                       | 0       |                                  |
| 38        | O            | O5          | 17                        | 0.085%                       | 0       |                                  |
| 38        | O            | O6          | 948                        | 4.739%                       | 1       |                                  |
| 38        | O            | O8          | 56                        | 0.280%                       | 0       |                                  |
| 43        | NE           | O6          | 99                        | 0.495%                       | 0       |                                  |
| 43        | NE           | O8          | 226                        | 1.130%                       | 0       |                                  |
| 43        | NE           | O13         | 32                        | 0.160%                       | 0       |                                  |
| 43        | NH1          | N54         | 1                         | 0.005%                       | 0       |                                  |
| 43        | NH1          | O4          | 44                        | 0.220%                       | 0       |                                  |
| 43        | NH1          | O5          | 8                         | 0.040%                       | 0       |                                  |
| 43        | NH1          | O6          | 113                        | 0.565%                       | 0       |                                  |
| 43        | NH1          | O7          | 8                         | 0.040%                       | 0       |                                  |
| 43        | NH1          | O8          | 616                        | 3.079%                       | 0       |                                  |
| 43        | NH1          | O10         | 7                         | 0.035%                       | 0       | 33.152%                          |
| 43        | NH1          | O13         | 147                        | 0.735%                       | 0       |                                  |
| 43        | NH2          | N54         | 1                         | 0.005%                       | 0       |                                  |
| 43        | NH2          | N55         | 1                         | 0.005%                       | 0       |                                  |
| 43        | NH2          | O4          | 6                         | 0.030%                       | 0       |                                  |
| 43        | NH2          | O5          | 74                        | 0.370%                       | 0       |                                  |
Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE |
|-----------|--------------|-------------|--------------------------|-------------------------------|---------|
| 43        | NH2          | O6          | 3492                     | 17.456%                       | 3       |
| 43        | NH2          | O7          | 62                       | 0.310%                        | 0       |
| 43        | NH2          | O8          | 1540                     | 7.698%                        | 1       |
| 43        | NH2          | O10         | 30                       | 0.150%                        | 0       |
| 43        | NH2          | O13         | 125                      | 0.625%                        | 0       |
| 48        | NE2          | O13         | 2                        | 0.010%                        | 0       |
| 48        | N            | O13         | 1                        | 0.005%                        | 0       |
| 48        | OE1          | N55         | 4                        | 0.020%                        | 0       |
| 48        | O            | N55         | 55                       | 0.275%                        | 0       |
| 48        | O            | O10         | 28                       | 0.140%                        | 0       |
| 48        | O            | O13         | 99                       | 0.495%                        | 0       |
| 50        | N            | O10         | 224                      | 1.120%                        | 0       |
| 50        | N            | O13         | 1275                     | 6.373%                        | 1       |
| 50        | OG1          | N55         | 20                       | 0.100%                        | 0       |
| 50        | OG1          | O10         | 697                      | 3.484%                        | 0       |
| 50        | OG1          | O13         | 704                      | 3.519%                        | 0       |
| 50        | O            | O10         | 3                        | 0.015%                        | 0       |
| 50        | O            | O13         | 24                       | 0.120%                        | 0       |
| 51        | N            | O13         | 1                        | 0.005%                        | 0       |
| 51        | O            | N55         | 2                        | 0.010%                        | 0       |
| 51        | O            | O13         | 1                        | 0.005%                        | 0       |
| 53        | O            | O13         | 1                        | 0.005%                        | 0       |
| 54        | N            | O11         | 2                        | 0.010%                        | 0       |
| 54        | O            | O10         | 13                       | 0.065%                        | 0       |
| 54        | O            | O11         | 121                      | 0.605%                        | 0       |
| 54        | O            | O12         | 125                      | 0.625%                        | 0       |
| 55        | NE2          | N54         | 2                        | 0.010%                        | 0       |
| 55        | NE2          | N55         | 18                       | 0.090%                        | 0       |
| 55        | NE2          | O10         | 257                      | 1.285%                        | 0       |
| 55        | NE2          | O11         | 145                      | 0.725%                        | 0       |
| 55        | NE2          | O12         | 72                       | 0.360%                        | 0       |
| 55        | NE2          | O13         | 55                       | 0.275%                        | 0       |
| 55        | N            | O10         | 80                       | 0.400%                        | 0       |
| 55        | N            | O12         | 1                        | 0.005%                        | 0       |
| 55        | N            | O13         | 1                        | 0.005%                        | 0       |
| 55        | OE1          | N54         | 1                        | 0.005%                        | 0       |
| 55        | OE1          | N55         | 688                      | 3.439%                        | 0       |
| 55        | OE1          | O10         | 381                      | 1.905%                        | 0       |
| 55        | OE1          | O11         | 31                       | 0.155%                        | 0       |
| 55        | OE1          | O12         | 22                       | 0.110%                        | 0       |
Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|--------------------------------|----------|------------------------------------|
| 55        | OE1          | O13         | 11                        | 0.055%                         | 0        |                                    |
| 55        | O            | N55         | 61                        | 0.305%                         | 0        |                                    |
| 55        | O            | O1          | 1                         | 0.005%                         | 0        |                                    |
| 55        | O            | O2          | 23                        | 0.115%                         | 0        |                                    |
| 55        | O            | O10         | 6831                      | 34.147%                        | 7        |                                    |
| 55        | O            | O11         | 62                        | 0.310%                         | 0        |                                    |
| 55        | O            | O12         | 10                        | 0.050%                         | 0        |                                    |
| 55        | O            | O13         | 3                         | 0.015%                         | 0        |                                    |
| 56        | N            | O10         | 96                        | 0.480%                         | 0        |                                    |
| 56        | N            | O11         | 1                         | 0.005%                         | 0        |                                    |
| 56        | O            | O11         | 24                        | 0.120%                         | 0        |                                    |
| 56        | O            | O12         | 1                         | 0.005%                         | 0        |                                    |
| 57        | N            | O2          | 6047                      | 30.227%                        | 6        | 30.232%                            |
| 58        | N            | O11         | 5                         | 0.025%                         | 0        |                                    |
| 58        | N            | O12         | 2                         | 0.010%                         | 0        |                                    |
| 58        | NZ           | O11         | 3                         | 0.015%                         | 0        |                                    |
| 58        | NZ           | O12         | 32                        | 0.160%                         | 0        |                                    |
| 60        | NE1          | O2          | 14                        | 0.070%                         | 0        |                                    |
| 60        | NE1          | O3          | 1194                      | 5.969%                         | 1        | 6.188%                             |
| 60        | NE1          | O4          | 30                        | 0.150%                         | 0        |                                    |
| 79        | NE2          | O12         | 1                         | 0.005%                         | 0        | 0.005%                             |
| 81        | O            | O12         | 1                         | 0.005%                         | 0        | 0.005%                             |
| 82        | O            | O3          | 199                       | 0.995%                         | 0        |                                    |
| 82        | O            | O4          | 1                         | 0.005%                         | 0        |                                    |
| 82        | O            | O11         | 16                        | 0.080%                         | 0        |                                    |
| 82        | O            | O12         | 27                        | 0.135%                         | 0        |                                    |
| 83        | OH           | O2          | 2                         | 0.010%                         | 0        |                                    |
| 83        | OH           | O3          | 710                       | 3.549%                         | 0        |                                    |
| 83        | OH           | O5          | 2                         | 0.010%                         | 0        |                                    |
| 83        | OH           | O7          | 27                        | 0.135%                         | 0        |                                    |
| 83        | OH           | O11         | 33                        | 0.165%                         | 0        | 5.379%                             |
| 83        | OH           | O12         | 115                       | 0.575%                         | 0        |                                    |
| 83        | OH           | O13         | 1                         | 0.005%                         | 0        |                                    |
| 83        | O            | O11         | 57                        | 0.285%                         | 0        |                                    |
| 83        | O            | O12         | 129                       | 0.645%                         | 0        |                                    |
| 84        | N            | O11         | 240                       | 1.200%                         | 0        |                                    |
| 84        | N            | O12         | 176                       | 0.880%                         | 0        | 3.424%                             |
| 84        | O            | O11         | 29                        | 0.145%                         | 0        |                                    |
| 84        | O            | O12         | 240                       | 1.200%                         | 0        |                                    |
Hydrogen bonds observed during last 400ns of MD simulations between Mc FKBP12 and APX879

| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|-------------------------------|---------|-----------------------------------|
| 85        | N            | O11         | 26                        | 0.130%                        | 0       |                                   |
| 85        | N            | O12         | 87                        | 0.435%                        | 0       |                                   |
| 85        | OE1          | O11         | 2                         | 0.010%                        | 0       |                                   |
| 85        | OE1          | O12         | 150                       | 0.750%                        | 0       |                                   |
| 85        | OE2          | O11         | 1                         | 0.005%                        | 0       | 2.224%                            |
| 85        | OE2          | O12         | 163                       | 0.815%                        | 0       |                                   |
| 85        | O            | O11         | 4                         | 0.020%                        | 0       |                                   |
| 85        | O            | O12         | 12                        | 0.060%                        | 0       |                                   |
| 86        | NE           | O11         | 42                        | 0.210%                        | 0       |                                   |
| 86        | NE           | O12         | 120                       | 0.600%                        | 0       |                                   |
| 86        | NE           | O13         | 2                         | 0.010%                        | 0       |                                   |
| 86        | NH1          | N54         | 1                         | 0.005%                        | 0       |                                   |
| 86        | NH1          | N55         | 1                         | 0.005%                        | 0       |                                   |
| 86        | NH1          | O11         | 86                        | 0.430%                        | 0       |                                   |
| 86        | NH1          | O12         | 213                       | 1.065%                        | 0       |                                   |
| 86        | NH1          | O13         | 10                        | 0.050%                        | 0       |                                   |
| 86        | NH2          | O11         | 52                        | 0.260%                        | 0       | 6.983%                            |
| 86        | NH2          | O12         | 126                       | 0.630%                        | 0       |                                   |
| 86        | NH2          | O13         | 7                         | 0.035%                        | 0       |                                   |
| 86        | N            | O11         | 38                        | 0.190%                        | 0       |                                   |
| 86        | N            | O12         | 454                       | 2.269%                        | 0       |                                   |
| 86        | O            | O10         | 4                         | 0.020%                        | 0       |                                   |
| 86        | O            | O11         | 65                        | 0.325%                        | 0       |                                   |
| 86        | O            | O12         | 175                       | 0.875%                        | 0       |                                   |
| 86        | O            | O13         | 1                         | 0.005%                        | 0       |                                   |
| 87        | N            | O11         | 110                       | 0.550%                        | 0       |                                   |
| 87        | N            | O12         | 76                        | 0.380%                        | 0       |                                   |
| 87        | O            | N55         | 6                         | 0.030%                        | 0       |                                   |
| 87        | O            | O10         | 2                         | 0.010%                        | 0       | 2.644%                            |
| 87        | O            | O11         | 103                       | 0.515%                        | 0       |                                   |
| 87        | O            | O12         | 231                       | 1.155%                        | 0       |                                   |
| 87        | O            | O13         | 1                         | 0.005%                        | 0       |                                   |
| 88        | N            | O10         | 505                       | 2.524%                        | 0       |                                   |
| 88        | N            | O11         | 19                        | 0.095%                        | 0       |                                   |
| 88        | N            | O12         | 144                       | 0.720%                        | 0       |                                   |
| 88        | N            | O13         | 3                         | 0.015%                        | 0       |                                   |
| 88        | OH           | N55         | 3                         | 0.015%                        | 0       |                                   |
| 88        | OH           | O3          | 1                         | 0.005%                        | 0       |                                   |
| 88        | OH           | O4          | 1                         | 0.005%                        | 0       |                                   |
| 88        | OH           | O5          | 1                         | 0.005%                        | 0       |                                   |
| Residue # | residue atom | APX879 atom | # of times hbond observed | frequency of hbond's existence | Z-SCORE | Overall residue frequency of hbonds |
|-----------|--------------|-------------|---------------------------|--------------------------------|---------|-----------------------------------|
| 88        | OH           | O6          | 11                        | 0.055%                         | 0       | 6.453%                            |
| 88        | OH           | O7          | 215                       | 1.075%                         | 0       |                                   |
| 88        | OH           | O8          | 1                         | 0.005%                         | 0       |                                   |
| 88        | OH           | O11         | 61                        | 0.305%                         | 0       |                                   |
| 88        | OH           | O12         | 131                       | 0.655%                         | 0       |                                   |
| 88        | OH           | O13         | 2                         | 0.010%                         | 0       |                                   |
| 88        | O            | O7          | 2                         | 0.010%                         | 0       |                                   |
| 88        | O            | O10         | 2                         | 0.010%                         | 0       |                                   |
| 88        | O            | O11         | 42                        | 0.210%                         | 0       |                                   |
| 88        | O            | O12         | 147                       | 0.735%                         | 0       |                                   |
| 89        | N            | O11         | 1                         | 0.005%                         | 0       |                                   |
| 89        | O            | O7          | 7                         | 0.035%                         | 0       |                                   |
| 89        | O            | O11         | 12                        | 0.060%                         | 0       |                                   |
| 89        | O            | O12         | 218                       | 1.090%                         | 0       | 1.190%                            |
| 90        | N            | O11         | 85                        | 0.425%                         | 0       |                                   |
| 90        | N            | O12         | 6                         | 0.030%                         | 0       | 0.600%                            |
| 90        | O            | O7          | 4                         | 0.020%                         | 0       |                                   |
| 90        | O            | O12         | 25                        | 0.125%                         | 0       |                                   |
| 91        | N            | O7          | 79                        | 0.395%                         | 0       |                                   |
| 91        | N            | O8          | 33                        | 0.165%                         | 0       |                                   |
| 91        | N            | O11         | 23                        | 0.115%                         | 0       |                                   |
| 91        | N            | O12         | 21                        | 0.105%                         | 0       |                                   |
| 91        | O            | O6          | 18                        | 0.090%                         | 0       | 1.105%                            |
| 91        | O            | O7          | 32                        | 0.160%                         | 0       |                                   |
| 91        | O            | O11         | 1                         | 0.005%                         | 0       |                                   |
| 91        | O            | O12         | 14                        | 0.070%                         | 0       |                                   |
| 92        | N            | O12         | 6                         | 0.030%                         | 0       | 0.060%                            |
| 92        | O            | O7          | 6                         | 0.030%                         | 0       |                                   |