

Supplementary file

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1 MUT protein main simulation data

In what follows we report tables showing the output of the *interactions vs time* addition. In each section we first provide a table with interactions sorted by the percentage in the START section, then we show another table with interactions sorted by the number of occurrences in all the frames. In each table the percentages above the threshold of 40% are underlined in bold. For the data regarding the pulling simulations, the percentages for the START, MIDDLE, END segments were 30%, 40%, 50%

1.1 MUT protein main simulation data - ligand

Interactions	Start	Middle	End	Frames
ALA191_B-GLN192_B	73.59%	0.0%	26.41%	231
MET49_A-TYR54_A	72.25%	27.62%	0.0%	782
ILE43_A-LEU57_A	58.58%	30.6%	10.82%	536
ARG188_B-LEU50_B	53.51%	39.47%	7.02%	114
ASN164_B-HSD163_B	52.14%	23.08%	24.79%	117
SER139_A-TYR126_A	50.5%	48.5%	0.0%	200
HSD41_B-CYS44_B	49.26%	25.56%	25.19%	270
LEU141_A-TYR118_A	48.21%	21.3%	30.04%	446
ILE43_B-LEU57_B	45.57%	27.09%	27.09%	406
SER144_A-HSD163_A	44.69%	25.22%	29.2%	226
SER144_B-HSD163_B	44.68%	24.82%	30.5%	282
LEU167_B-ALA194_B	43.54%	27.68%	28.6%	542
LEU167_A-PHE185_A	42.82%	30.96%	26.08%	717
SER139_A-ARG4_B	42.74%	26.61%	30.65%	248
LEU167_B-PHE185_B	41.68%	34.35%	23.97%	559
THR26_A-THR21_A	40.9%	36.17%	22.71%	951
THR25_A-CYS44_A	36.2%	23.54%	40.25%	790
THR45_A-ASP48_A	33.8%	18.05%	47.99%	1219
THR26_B-THR21_B	33.45%	45.3%	21.08%	574
VAL42_B-GLY23_B	24.62%	3.9%	71.47%	333
VAL42_A-VAL20_A	24.24%	22.04%	53.72%	363
ASN164_A-THR175_A	24.09%	45.26%	30.66%	137
THR26_A-GLN19_A	23.64%	56.36%	20.0%	165
VAL42_B-LEU27_B	23.5%	27.24%	49.02%	1230
ASP48_A-ASN51_A	22.55%	37.25%	40.2%	204
ILE43_B-LEU58_B	22.31%	18.73%	58.96%	251
VAL42_B-VAL20_B	22.09%	17.67%	60.24%	249
ASP48_B-ASN51_B	21.97%	13.64%	64.39%	132
ASP187_B-TYR54_B	20.61%	34.47%	44.82%	1082
ILE43_A-LYS61_A	12.45%	13.73%	73.82%	233
GLU166_A-SER307_A	8.1%	61.11%	30.79%	630
LEU167_A-ALA194_A	3.03%	45.76%	51.21%	330
PHE140_A-SER307_A	2.7%	74.32%	22.3%	148
ARG188_A-PRO52_A	0.57%	43.91%	55.24%	353
ASP48_A-LYS61_A	0.18%	14.76%	85.06%	542
TYR54_A-ASP187_A	0.12%	36.76%	62.99%	816
THR190_A-VAL186_A	0.0%	77.48%	21.85%	151
MET49_A-ARG188_A	0.0%	42.45%	57.37%	563
ARG188_A-ASN51_A	0.0%	50.97%	49.03%	463
THR25_A-THR21_A	0.0%	24.74%	75.26%	190

Table 1: The following table has been obtained analyzing the data relative to the residues interacting with the **Ligand**. We remind that those residues are responsible for the association and dissociation of the ligand to the protein. Also, the residues at a lower distance than 6 Å were considered.

Interactions	Start	Middle	End	Frames
VAL42_B-LEU27_B	23.5%	27.24%	49.02%	1230
THR45_A-ASP48_A	33.8%	18.05%	47.99%	1219
ASP187_B-TYR54_B	20.61%	34.47%	44.82%	1082
THR26_A-THR21_A	40.9%	36.17%	22.71%	951
TYR54_A-ASP187_A	0.12%	36.76%	62.99%	816
THR25_A-CYS44_A	36.2%	23.54%	40.25%	790
MET49_A-TYR54_A	72.25%	27.62%	0.0%	782
LEU167_A-PHE185_A	42.82%	30.96%	26.08%	717
ASP48_A-LYS61_A	0.15%	15.07%	84.78%	670
GLU166_A-SER1_B	8.1%	61.11%	30.79%	630
THR26_B-THR21_B	33.45%	45.3%	21.08%	574
MET49_A-ARG188_A	0.0%	42.45%	57.37%	563
LEU167_B-PHE185_B	41.68%	34.35%	23.97%	559
LEU167_B-ALA194_B	43.54%	27.68%	28.6%	542
ILE43_A-LEU57_A	58.58%	30.6%	10.82%	536
ARG188_A-ASN51_A	0.0%	50.97%	49.03%	463
LEU141_A-TYR118_A	48.21%	21.3%	30.04%	446
ILE43_B-LEU57_B	45.57%	27.09%	27.09%	406
VAL42_A-VAL20_A	24.24%	22.04%	53.72%	363
ARG188_A-PRO52_A	0.57%	43.91%	55.24%	353
VAL42_B-GLY23_B	24.62%	3.9%	71.47%	333
LEU167_A-ALA194_A	3.03%	45.76%	51.21%	330
SER144_B-HSD163_B	44.68%	24.82%	30.5%	282
HSD41_B-CYS44_B	49.26%	25.56%	25.19%	270
ILE43_B-LEU58_B	22.31%	18.73%	58.96%	251
VAL42_B-VAL20_B	22.09%	17.67%	60.24%	249
SER139_A-ARG4_B	42.74%	26.61%	30.65%	248
ILE43_A-LYS61_A	12.45%	13.73%	73.82%	233
ALA191_B-GLN192_B	73.59%	0.0%	26.41%	231
SER144_A-HSD163_A	44.69%	25.22%	29.2%	226
ASP48_A-ASN51_A	22.55%	37.25%	40.2%	204
SER139_A-TYR126_A	50.5%	48.5%	0.0%	200
THR25_A-THR21_A	0.0%	24.74%	75.26%	190
THR26_A-GLN19_A	23.64%	56.36%	20.0%	165
THR190_A-VAL186_A	0.0%	77.48%	21.85%	151
PHE140_A-SER307_A	2.7%	74.32%	22.3%	148
ASN164_A-THR175_A	24.09%	45.26%	30.66%	137
ASP48_B-ASN51_B	21.97%	13.64%	64.39%	132
ASN164_B-HSD163_B	52.14%	23.08%	24.79%	117
ARG188_B-LEU50_B	53.51%	39.47%	7.02%	114

Table 2: Interactions sorted by number of frames for the ligand residues of MUT.

1.1.1 Bar plots for the ligand residues with four sorting methods

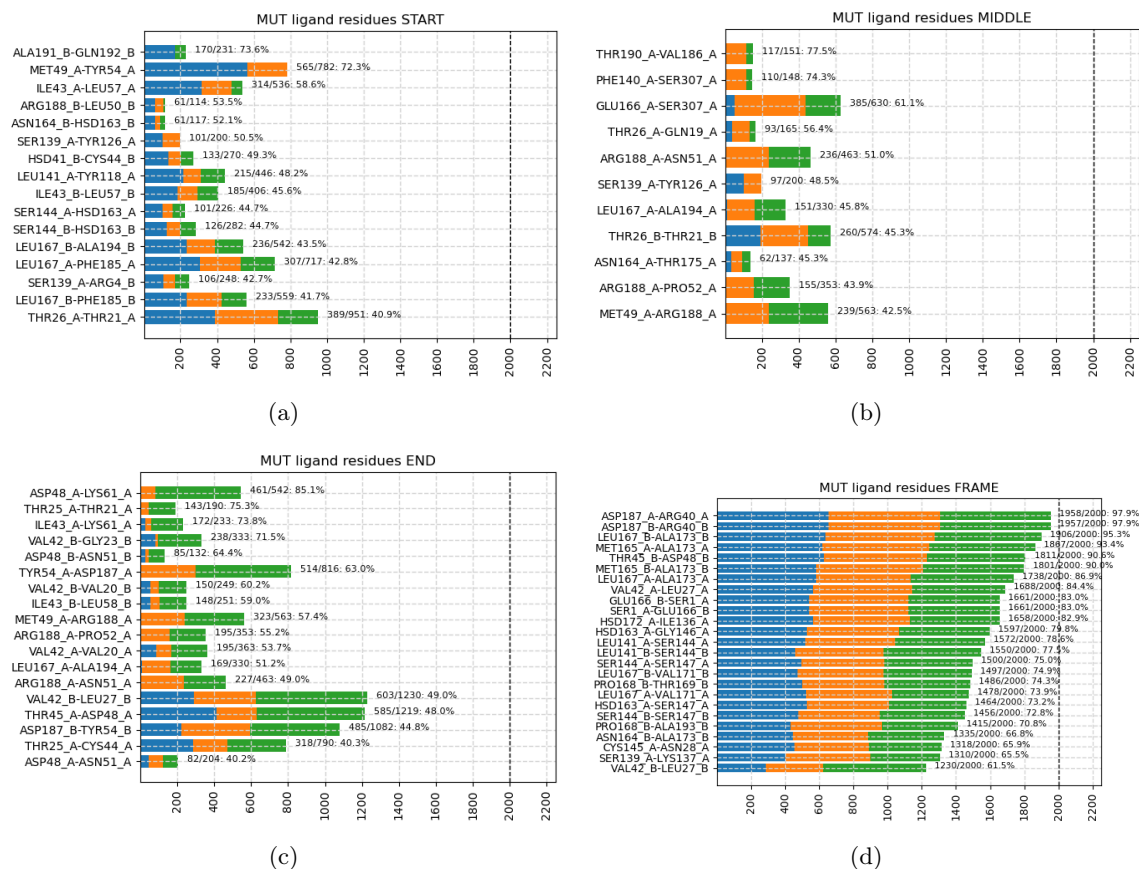


Figure 1: MUT protein, bar plots of the interactions involving residues interacting with the ligand. Each graph lists the interactions with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). We estimated a cut-off of 40% to consider an interaction particularly present in a specific portion of the trajectory

1.2 MUT protein main simulation data - dimerization

Interactions	Start	Middle	End	Frames
SER1_A-PHE140_B	87.85%	5.67%	6.48%	247
MET6_A-GLN299_A	81.55%	15.45%	3.0%	233
ARG4_A-GLN299_A	71.91%	21.28%	6.6%	470
ARG298_B-GLY302_B	57.14%	40.48%	2.38%	168
ARG298_B-ASP295_B	51.53%	22.09%	25.77%	163
LYS5_A-GLU290_A	51.24%	3.92%	44.84%	1046
SER139_A-TYR126_A	50.5%	48.5%	0.0%	200
MET6_A-ALA116_B	49.9%	22.14%	27.86%	980
ALA7_A-ALA7_B	47.26%	45.89%	6.16%	146
PHE3_A-VAL296_A	43.02%	38.99%	17.81%	1067
SER139_A-ARG4_B	42.74%	26.61%	30.65%	248
ALA7_A-VAL125_B	40.02%	30.45%	29.46%	1317
CYS300_B-VAL296_B	38.71%	51.57%	9.39%	607
CYS22_B-THR25_B	33.21%	44.47%	22.33%	533
PHE3_A-ARG4_A	31.23%	8.66%	59.97%	762
MET6_B-ALA116_A	26.52%	51.65%	21.49%	577
CYS85_B-ARG40_B	21.55%	25.0%	53.45%	116
ARG298_A-VAL303_A	8.7%	12.42%	78.88%	161
GLU166_A-SER307_A	8.1%	61.11%	30.79%	630
GLU290_B-LYS137_B	4.53%	82.62%	12.59%	397
GLU290_A-LYS137_A	3.97%	76.68%	19.17%	579

Table 3: The following table has been obtained analyzing the data relative to the residues responsible for a correct **dimerization** of the MUT protein. All the amino acids are numbered starting from 1 to the total length of a monomer.

Interactions	Start	Middle	End	Frames
ARG298_B-ASP295_B	42.82%	32.83%	24.19%	1261
PHE3_A-VAL296_A	43.02%	38.99%	17.81%	1067
LYS5_A-GLU290_A	51.24%	3.92%	44.84%	1046
MET6_A-ALA116_B	49.9%	22.14%	27.86%	980
GLU290_A-LYS137_A	3.84%	76.73%	19.05%	782
PHE3_A-ARG4_A	31.23%	8.66%	59.97%	762
GLU166_A-SER307_A	8.1%	61.11%	30.79%	630
CYS300_B-VAL296_B	38.71%	51.57%	9.39%	607
MET6_B-ALA116_A	26.52%	51.65%	21.49%	577
CYS22_B-THR25_B	33.21%	44.47%	22.33%	533
GLU290_B-LYS137_B	3.82%	82.93%	13.05%	498
ARG4_A-GLN299_A	71.91%	21.28%	6.6%	470
SER139_A-ARG4_B	42.74%	26.61%	30.65%	248
SER1_A-PHE140_B	87.85%	5.67%	6.48%	247
MET6_A-GLN299_A	81.55%	15.45%	3.0%	233
SER139_A-TYR126_A	50.5%	48.5%	0.0%	200
ARG298_B-GLY302_B	57.14%	40.48%	2.38%	168
ARG298_A-VAL303_A	8.7%	12.42%	78.88%	161
ALA7_A-ALA7_B	47.26%	45.89%	6.16%	146
CYS85_B-ARG40_B	21.55%	25.0%	53.45%	116

Table 4: Interactions sorted by number of frames for the **dimerization** residues of MUT.

1.2.1 Bar plots for the dimerization residues with four sorting methods

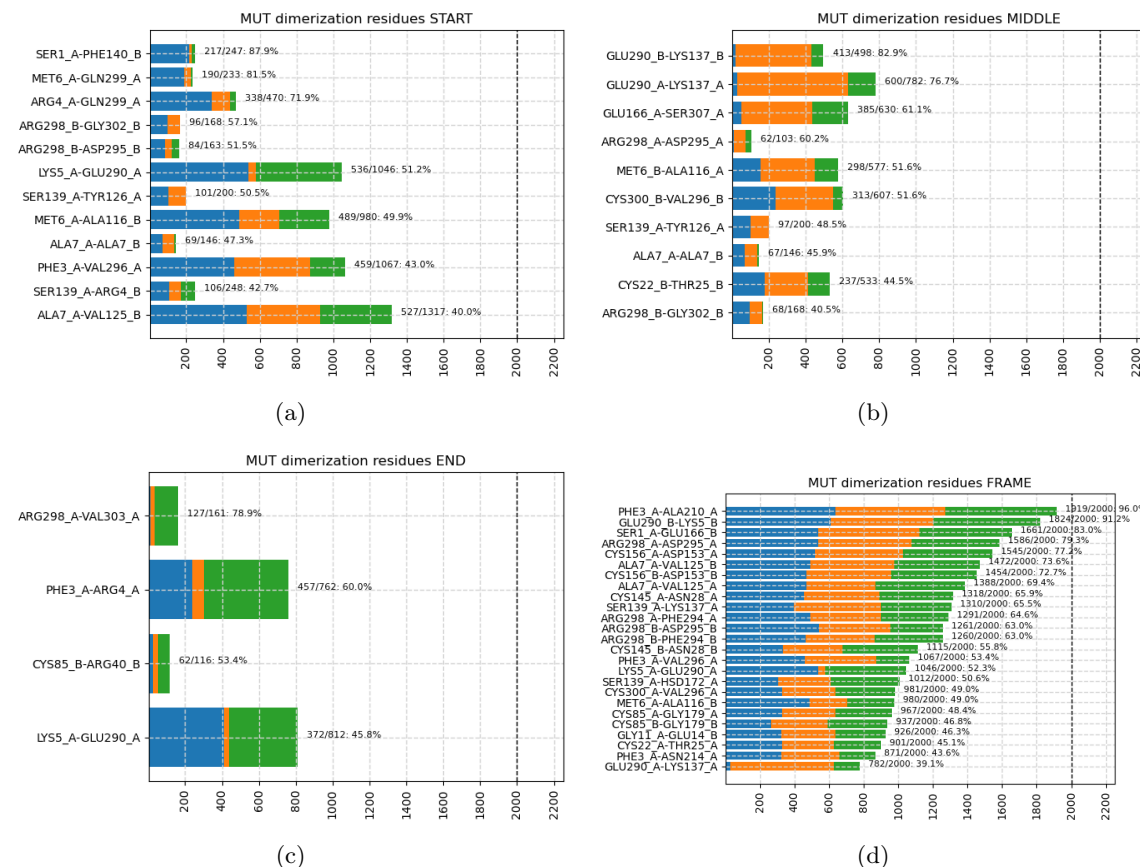


Figure 2: MUT protein, bar plots of the interactions involving residues for the **dimerization**. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). We considered a cut-off of 40%.

1.3 MUT protein pulling simulation - ligand

Interactions	Start	Middle	End	Frames
THR25_A-CYS44_A	31.25%	31.25%	36.54%	208
ARG188_A-ASN51_A	30.0%	31.25%	38.75%	80
HSD41_A-ASN164_A	19.7%	30.3%	50.0%	66
THR190_A-GLN192_A	11.11%	51.11%	37.78%	45
ASP48_A-ASN51_A	10.11%	44.94%	44.94%	89
MET49_A-PRO52_A	1.37%	42.47%	56.16%	73

Table 5: MUT protein, ligand interactions, interactions sorted by the **Start** section.

Interactions	Start	Middle	End	Frames
THR25_A-CYS44_A	31.25%	31.25%	36.54%	208
ASP48_A-ASN51_A	10.11%	44.94%	44.94%	89
ARG188_A-ASN51_A	30.0%	31.25%	38.75%	80
MET49_A-PRO52_A	1.37%	42.47%	56.16%	73
HSD41_A-ASN164_A	19.7%	30.3%	50.0%	66
THR190_A-GLN192_A	11.11%	51.11%	37.78%	45

Table 6: MUT protein, ligand interactions, interactions sorted by the **Frames** section.

1.3.1 MUT pulling: Bar plots for the ligand residues with four sorting methods

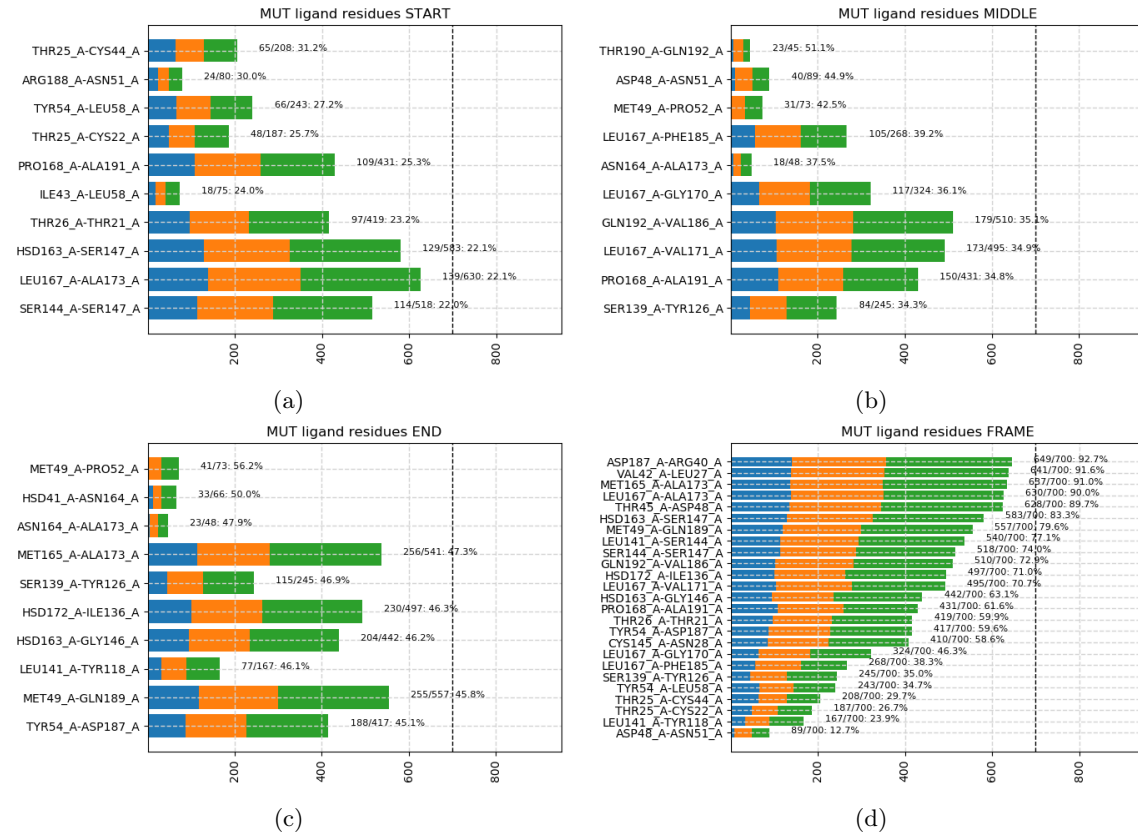


Figure 3: MUT protein, bar plots of the interactions involving residues of the **Ligand** residues. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered cut-offs of 30% for the "START" section, 40% for the "MIDDLE" section and 50% for the "END" section.

1.4 MUT protein pulling simulation - dimerization

Interactions	Start	Middle	End	Frames
LYS5_A-GLN127_A	100.0%	0.0%	0.0%	46
GLY2_A-ASN214_A	48.15%	25.93%	25.93%	81
PHE3_A-LEU282_A	31.65%	29.11%	39.24%	79
LYS5_A-GLU288_A	0.35%	35.29%	64.01%	289
PHE3_A-ARG4_A	0.0%	13.21%	86.79%	53

Table 7: MUT protein, **dimerization** interactions, interactions sorted by the **Start** section.

Interactions	Start	Middle	End	Frames
LYS5_A-GLU288_A	0.24%	39.12%	60.39%	409
GLY2_A-ASN214_A	48.15%	25.93%	25.93%	81
PHE3_A-LEU282_A	31.65%	29.11%	39.24%	79
PHE3_A-ARG4_A	0.0%	13.21%	86.79%	53
LYS5_A-GLN127_A	100.0%	0.0%	0.0%	46

Table 8: MUT protein, **dimerization** interactions, interactions sorted by the **Frames** section.

1.4.1 MUT protein pulling. Bar plots for the dimerization residues with four sorting methods

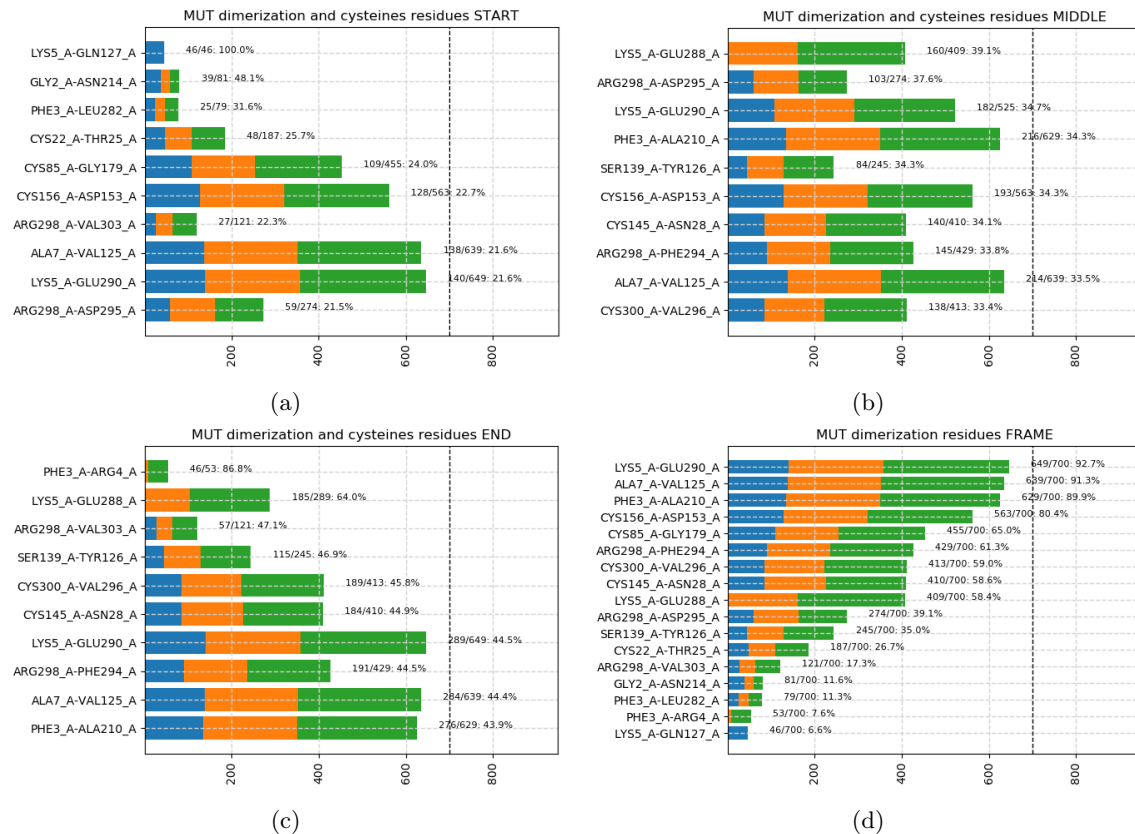


Figure 4: MUT protein, bar plots of the interactions involving residues of the **Dimerization** selection. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered cut-offs of 30% for the "START" section, 40% for the "MIDDLE" section and 50% for the "END" section.

2 WT protein main simulation data

2.1 WT protein main simulation data - ligand

Interactions	Start	Middle	End	Frames
THR45_B-ASP48_B	100.0%	0.0%	0.0%	431
SER144_A-CYS117_A	100.0%	0.0%	0.0%	777
MET49_A-GLN189_A	99.83%	0.17%	0.0%	587
LEU167_A-GLY170_A	99.43%	0.0%	0.57%	526
HSD41_A-HSD164_A	98.14%	0.0%	1.86%	429
MET49_B-GLN189_B	97.55%	0.2%	2.25%	1021
PRO168_B-ALA193_B	79.84%	19.1%	1.06%	377
THR26_A-GLN19_A	69.74%	16.88%	13.39%	717
GLN192_A-VAL186_A	66.17%	26.48%	7.27%	1348
PRO168_A-ALA193_A	64.77%	8.07%	27.16%	545
LEU167_A-PHE185_A	62.03%	29.06%	8.91%	561
GLN192_B-VAL186_B	61.34%	38.56%	0.0%	2059
ASP187_A-ARG40_A	59.11%	12.81%	28.05%	2998
TYR54_A-ASP187_A	51.83%	41.53%	6.64%	2273
THR25_A-CYS22_A	51.56%	28.39%	19.99%	1761
PRO168_A-ALA191_A	49.51%	13.03%	36.81%	307
LEU167_B-ALA194_B	47.73%	20.0%	32.27%	970
THR26_A-THR21_A	46.64%	33.39%	19.97%	1743
GLY143_B-ASN28_B	44.34%	29.79%	25.64%	433
HSD164_B-ALA173_B	44.32%	29.85%	25.64%	546
SER139_B-GLN299_A	41.86%	46.72%	11.36%	1541
THR190_B-GLN192_B	41.37%	42.67%	15.96%	307
THR25_A-CYS44_A	36.96%	17.1%	45.94%	579
VAL42_B-LEU27_B	36.36%	22.93%	40.63%	3955
ARG4_B-GLU290_A	31.58%	23.57%	44.85%	1523
GLU290_A-ARG4_B	31.58%	23.57%	44.85%	1523
ILE43_B-LEU57_B	31.24%	21.85%	46.91%	1245
SER139_B-GLY2_A	28.99%	29.74%	41.24%	2791
THR190_A-GLN192_A	28.34%	43.02%	28.49%	688
VAL42_B-VAL20_B	27.34%	41.99%	30.66%	512
ASP187_B-TYR54_B	26.54%	27.91%	45.5%	2035
MET49_B-PRO52_B	26.45%	65.84%	7.71%	1452
SER139_A-TYR126_A	25.8%	51.29%	22.91%	659
VAL42_A-VAL20_A	25.75%	17.47%	56.78%	435
GLU166_A-HSD172_A	25.59%	16.13%	58.28%	465
HSD164_A-THR175_A	25.53%	33.46%	41.01%	1034

Table 9: WT protein, residues interacting with the **ligand**. The interactions are sorted on the base of the values in the **Start** column - 1st part of the table.

Interactions	Start	Middle	End	Frames
ILE43_A-LEU58_A	25.44%	43.38%	31.18%	574
THR26_B-THR21_B	24.35%	33.65%	42.0%	1881
LEU167_B-PHE185_B	21.87%	29.33%	48.74%	1623
ILE43_A-LEU57_A	21.43%	21.71%	56.86%	1465
SER139_A-ARG4_B	19.51%	42.94%	37.48%	1374
LEU141_A-SER144_A	19.15%	41.65%	39.11%	3186
HSD163_A-GLY146_A	18.39%	43.88%	37.61%	2648
PRO168_A-THR169_A	17.01%	43.52%	39.38%	3433
HSD172_A-SER1_B	16.36%	62.14%	21.42%	1186
SER144_A-SER147_A	16.33%	41.96%	41.67%	4183
ILE43_B-LEU58_B	14.72%	65.09%	20.07%	822
PHE140_A-GLY2_B	14.04%	44.75%	41.14%	2941
ASP48_A-LYS61_A	13.0%	84.05%	2.95%	746
ASN142_A-SER301_B	12.11%	44.07%	43.83%	413
ALA193_A-PRO184_A	12.09%	71.39%	16.22%	339
PHE140_A-GLN299_B	11.34%	56.37%	32.29%	1728
MET49_A-ARG188_A	11.25%	58.39%	30.36%	471
THR25_A-THR21_A	10.27%	32.62%	57.04%	1597
PHE140_A-PHE3_B	10.26%	27.86%	61.88%	585
ASN142_A-GLN299_B	9.79%	36.32%	53.84%	1798
ARG188_B-LEU50_B	6.96%	0.0%	93.04%	790
ASP48_B-GLN189_B	4.14%	39.81%	56.05%	314
THR45_B-LYS61_B	2.44%	92.91%	4.65%	409
VAL42_A-GLY23_A	2.22%	17.41%	80.38%	586
MET49_A-TYR54_A	1.99%	4.86%	93.15%	1256
CYS44_A-THR24_A	0.93%	18.94%	80.12%	322
ASP187_A-ARG188_A	0.8%	60.62%	38.51%	1615
ASN142_A-CYS300_B	0.33%	39.1%	60.57%	908
MET49_A-LEU50_A	0.31%	9.23%	90.46%	325
MET49_B-LEU50_B	0.0%	1.09%	98.91%	824
SER46_B-ARG188_B	0.0%	0.0%	100.0%	797
THR190_B-VAL186_B	0.0%	0.0%	100.0%	343
GLU47_B-LEU50_B	0.0%	0.0%	100.0%	314
VAL42_A-THR24_A	0.0%	98.31%	1.69%	356

Table 10: WT protein, residues interacting with the **ligand**. The interactions are sorted on the base of the values in the **Start** column - 2nd part of the table.

Interactions	Start	Middle	End	Frames
SER144_A-SER147_A	16.33%	41.96%	41.67%	4183
VAL42_B-LEU27_B	36.36%	22.93%	40.63%	3955
PRO168_A-THR169_A	17.01%	43.52%	39.38%	3433
ASP187_A-ARG40_A	54.75%	18.96%	26.24%	3297
LEU141_A-SER144_A	19.15%	41.65%	39.11%	3186
PHE140_A-GLY2_B	14.04%	44.75%	41.14%	2941
SER139_B-GLY2_A	28.99%	29.74%	41.24%	2791
HSD163_A-GLY146_A	18.39%	43.88%	37.61%	2648
TYR54_A-ASP187_A	51.83%	41.53%	6.64%	2273
GLN192_B-VAL186_B	61.34%	38.56%	0.0%	2059
ASP187_B-TYR54_B	26.54%	27.91%	45.5%	2035
THR26_B-THR21_B	24.35%	33.65%	42.0%	1881
ASN142_A-GLN299_B	9.79%	36.32%	53.84%	1798
THR25_A-CYS22_A	51.56%	28.39%	19.99%	1761
THR26_A-THR21_A	46.64%	33.39%	19.97%	1743
PHE140_A-GLN299_B	11.34%	56.37%	32.29%	1728
LEU167_B-PHE185_B	21.87%	29.33%	48.74%	1623
ASP187_A-ARG188_A	0.19%	64.65%	35.1%	1621
THR25_A-THR21_A	10.27%	32.62%	57.04%	1597
SER139_B-GLN299_A	41.86%	46.72%	11.36%	1541
ILE43_A-LEU57_A	21.43%	21.71%	56.86%	1465
MET49_B-PRO52_B	26.45%	65.84%	7.71%	1452
SER139_A-ARG4_B	19.51%	42.94%	37.48%	1374
GLN192_A-VAL186_A	66.17%	26.48%	7.27%	1348
MET49_A-TYR54_A	1.99%	4.86%	93.15%	1256
ILE43_B-LEU57_B	31.24%	21.85%	46.91%	1245
HSD172_A-SER1_B	16.36%	62.14%	21.42%	1186
HSD164_A-THR175_A	25.53%	33.46%	41.01%	1034
MET49_B-GLN189_B	97.55%	0.2%	2.25%	1021
LEU167_B-ALA194_B	47.73%	20.0%	32.27%	970
ASN142_A-CYS300_B	0.33%	39.1%	60.57%	908
ASP48_A-LYS61_A	12.98%	84.12%	2.91%	894
MET49_B-LEU50_B	0.0%	1.09%	98.91%	824
ILE43_B-LEU58_B	14.72%	65.09%	20.07%	822
SER46_B-ARG188_B	0.0%	0.0%	100.0%	797
ARG188_B-LEU50_B	6.96%	0.0%	93.04%	790
SER144_A-CYS117_A	100.0%	0.0%	0.0%	777
THR26_A-GLN19_A	69.74%	16.88%	13.39%	717
THR190_A-GLN192_A	28.34%	43.02%	28.49%	688
SER139_A-TYR126_A	25.8%	51.29%	22.91%	659
MET49_A-GLN189_A	99.83%	0.17%	0.0%	587
VAL42_A-GLY23_A	2.22%	17.41%	80.38%	586
PHE140_A-PHE3_B	10.26%	27.86%	61.88%	585
THR25_A-CYS44_A	36.96%	17.1%	45.94%	579
ILE43_A-LEU58_A	25.44%	43.38%	31.18%	574
LEU167_A-PHE185_A	62.03%	29.06%	8.91%	561
HSD164_B-ALA173_B	44.32%	29.85%	25.64%	546
PRO168_A-ALA193_A	64.77%	8.07%	27.16%	545
LEU167_A-GLY170_A	99.43%	0.0%	0.57%	526

Table 11: WT interactions involving residues in communication with the **ligand**. - 1st part of the table. The interactions are ordered based on the number of frames.

Interactions	Start	Middle	End	Frames
VAL42_B-VAL20_B	27.34%	41.99%	30.66%	512
MET49_A-ARG188_A	11.25%	58.39%	30.36%	471
GLU166_A-HSD172_A	25.59%	16.13%	58.28%	465
VAL42_A-VAL20_A	25.75%	17.47%	56.78%	435
GLY143_B-ASN28_B	44.34%	29.79%	25.64%	433
THR45_B-ASP48_B	100.0%	0.0%	0.0%	431
HSD41_A-HSD164_A	98.14%	0.0%	1.86%	429
ASN142_A-SER301_B	12.11%	44.07%	43.83%	413
THR45_B-LYS61_B	2.44%	92.91%	4.65%	409
PRO168_B-ALA193_B	79.84%	19.1%	1.06%	377
VAL42_A-THR24_A	0.0%	98.31%	1.69%	356
THR190_B-VAL186_B	0.0%	0.0%	100.0%	343
ALA193_A-PRO184_A	12.09%	71.39%	16.22%	339
MET49_A-LEU50_A	0.31%	9.23%	90.46%	325
CYS44_A-THR24_A	0.93%	18.94%	80.12%	322
ASP48_B-GLN189_B	4.14%	39.81%	56.05%	314
GLU47_B-LEU50_B	0.0%	0.0%	100.0%	314
THR190_B-GLN192_B	41.37%	42.67%	15.96%	307
PRO168_A-ALA191_A	49.51%	13.03%	36.81%	307

Table 12: WT interactions involving residues in communication with the **ligand**. - 2nd part of the table.

2.1.1 WT: Bar plots for the ligand residues with four sorting methods

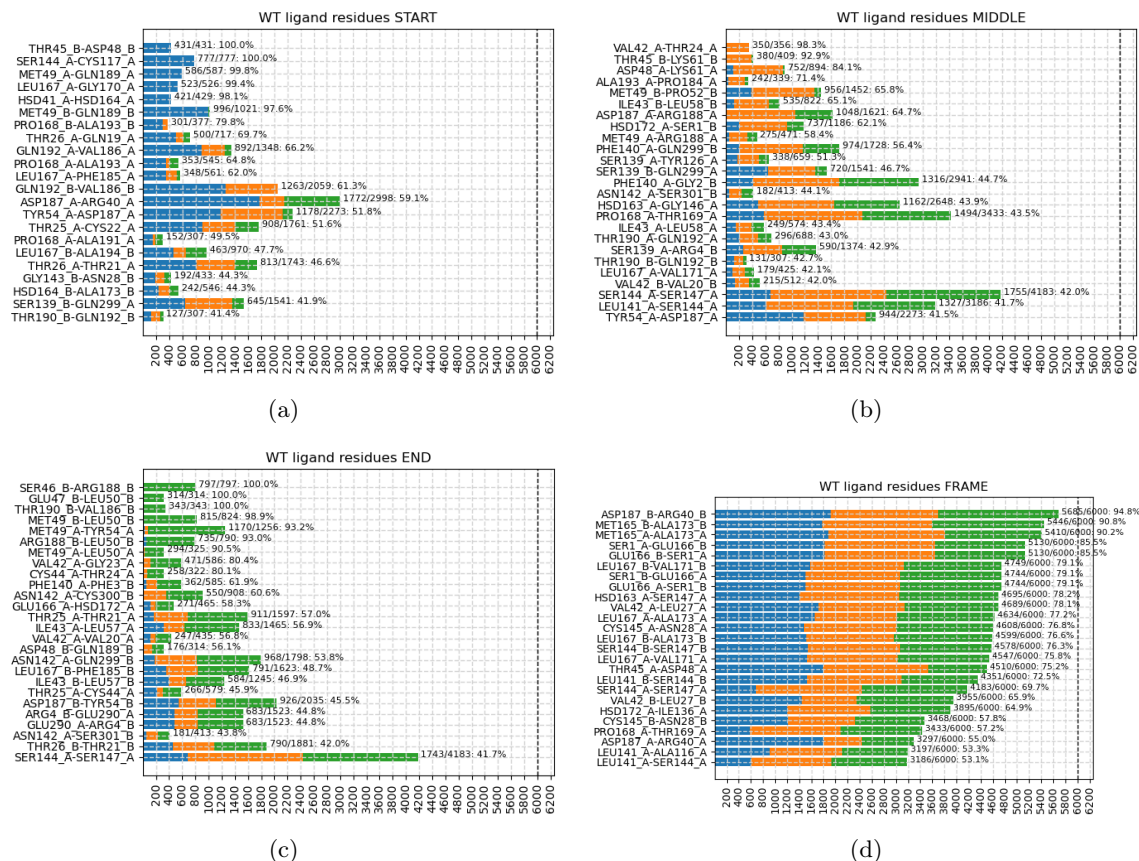


Figure 5: WT protein, bar plots of the interactions involving residues in connection with the **ligand**. Each graph lists the bonds with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered a cut-off of 40% to retain significant an interaction.

2.2 WT protein main simulation data - dimerization

Interactions	Start	Middle	End	Frames
GLU290_A-ARG131_A	94.14%	3.7%	1.85%	324
GLU290_A-ALA129_A	72.33%	1.17%	26.5%	600
CYS300_A-VAL296_A	68.86%	11.6%	19.54%	1095
PHE3_A-LEU282_A	65.97%	20.93%	13.1%	626
CYS300_B-VAL296_B	59.68%	24.46%	15.78%	1198
PHE3_A-PHE291_A	56.79%	34.81%	8.41%	928
ALA7_A-ALA7_B	52.99%	24.88%	22.14%	402
CYS22_A-THR25_A	51.56%	28.39%	19.99%	1761
ARG4_A-LYS137_B	47.0%	1.04%	51.96%	383
CYS85_B-ARG40_B	44.42%	33.26%	22.09%	430
MET6_A-GLN127_A	42.25%	20.35%	37.21%	516
SER139_B-GLN299_A	41.86%	46.72%	11.36%	1541
ARG298_A-PHE294_A	40.26%	32.43%	27.31%	2263
ARG4_A-GLN299_A	34.47%	54.55%	10.88%	1958
ARG4_B-GLU290_A	31.58%	23.57%	44.85%	1523
GLU290_A-ARG4_B	31.58%	23.57%	44.85%	1523
GLY2_A-SER139_B	28.99%	29.74%	41.24%	2791
GLU290_B-GLN127_B	27.0%	48.45%	24.49%	1674
SER139_A-TYR126_A	25.8%	51.29%	22.91%	659
GLU166_A-HSD172_A	25.59%	16.13%	58.28%	465
MET6_A-ALA116_B	23.52%	25.59%	50.89%	1012
SER139_A-ARG4_B	19.51%	42.94%	37.48%	1374
ARG298_B-ASP295_B	18.14%	37.43%	44.4%	2525
GLU290_B-GLU288_B	15.51%	52.88%	31.61%	503
MET6_B-ALA116_A	15.1%	44.62%	40.28%	1358
ARG298_A-ASP295_A	14.86%	35.22%	49.92%	1238
ASN142_A-SER301_B	12.11%	44.07%	43.83%	413
ASN142_A-GLN299_B	9.79%	36.32%	53.84%	1798
CYS44_A-THR24_A	0.93%	18.94%	80.12%	322
ASN142_A-CYS300_B	0.33%	39.1%	60.57%	908

Table 13: WT residues for **dimerization**

Interactions	Start	Middle	End	Frames
GLY2_A-SER139_B	28.99%	29.74%	41.24%	2791
ARG298_B-ASP295_B	18.14%	37.43%	44.4%	2525
ARG298_A-PHE294_A	40.26%	32.43%	27.31%	2263
ARG4_A-GLN299_A	34.47%	54.55%	10.88%	1958
ASN142_A-GLN299_B	9.79%	36.32%	53.84%	1798
CYS22_A-THR25_A	51.56%	28.39%	19.99%	1761
GLU290_B-GLN127_B	27.0%	48.45%	24.49%	1674
SER139_B-GLN299_A	41.86%	46.72%	11.36%	1541
SER139_A-ARG4_B	19.51%	42.94%	37.48%	1374
MET6_B-ALA116_A	15.1%	44.62%	40.28%	1358
ARG298_A-ASP295_A	14.86%	35.22%	49.92%	1238
CYS300_B-VAL296_B	59.68%	24.46%	15.78%	1198
CYS300_A-VAL296_A	68.86%	11.6%	19.54%	1095
MET6_A-ALA116_B	23.52%	25.59%	50.89%	1012
PHE3_A-PHE291_A	56.79%	34.81%	8.41%	928
ASN142_A-CYS300_B	0.33%	39.1%	60.57%	908
SER139_A-TYR126_A	25.8%	51.29%	22.91%	659
PHE3_A-LEU282_A	65.97%	20.93%	13.1%	626
GLU290_A-ALA129_A	72.33%	1.17%	26.5%	600
MET6_A-GLN127_A	42.25%	20.35%	37.21%	516
GLU290_B-GLU288_B	15.51%	52.88%	31.61%	503
GLU166_A-HSD172_A	25.59%	16.13%	58.28%	465
CYS85_B-ARG40_B	44.42%	33.26%	22.09%	430
ASN142_A-SER301_B	12.11%	44.07%	43.83%	413
ALA7_A-ALA7_B	52.99%	24.88%	22.14%	402
ARG4_A-LYS137_B	47.0%	1.04%	51.96%	383
GLU290_A-ARG131_A	94.14%	3.7%	1.85%	324
CYS44_A-THR24_A	0.93%	18.94%	80.12%	322

Table 14: WT interactions involving residues for the **dimerization**.

2.2.1 WT protein: bar plots for the dimerization residues with four sorting methods

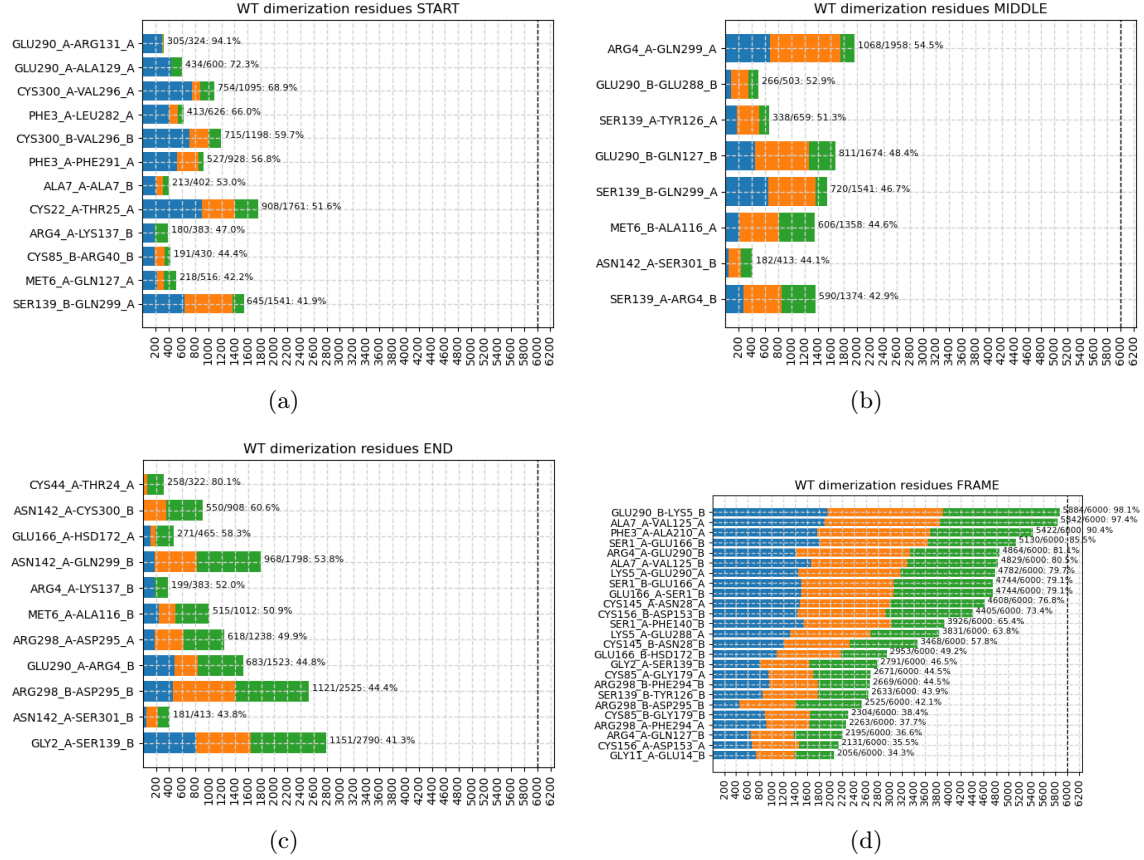


Figure 6: WT protein, bar plots of the interactions involving residues for **dimerization**. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered a cut-off of 40%.

2.3 WT pulling simulation - ligand

Interactions	Start	Middle	End	Frames
SER144_A-HSD163_A	59.06%	18.11%	22.83%	127
ILE43_A-LEU57_A	30.56%	16.67%	50.0%	36
ASP48_A-ASN51_A	18.75%	31.25%	50.0%	48
LEU167_A-GLY170_A	18.31%	27.46%	54.23%	142
HSD41_A-CYS44_A	15.97%	25.21%	58.82%	119
ARG188_A-THR190_A	10.0%	36.67%	52.22%	90
HSD163_A-TYR161_A	4.8%	41.6%	53.6%	125
LEU141_A-SER144_A	4.38%	43.43%	51.18%	297
SER46_A-GLU47_A	0.0%	64.9%	35.1%	151

Table 15: WT protein, **ligand** interactions in the pulling simulation. Sorting method: **Start**.

Interactions	Start	Middle	End	Frames
LEU141_A-SER144_A	4.38%	43.43%	51.18%	297
SER46_A-GLU47_A	0.0%	64.9%	35.1%	151
LEU167_A-GLY170_A	18.31%	27.46%	54.23%	142
SER144_A-HSD163_A	59.06%	18.11%	22.83%	127
HSD163_A-TYR161_A	4.8%	41.6%	53.6%	125
HSD41_A-CYS44_A	15.97%	25.21%	58.82%	119
ARG188_A-THR190_A	10.0%	36.67%	52.22%	90
ASP48_A-ASN51_A	18.75%	31.25%	50.0%	48
ILE43_A-LEU57_A	30.56%	16.67%	50.0%	36

Table 16: WT protein, **ligand** interactions in the pulling simulation. Sorting method: **Frames**.

2.3.1 WT protein pulling. Bar plots for the ligand residues with four sorting methods

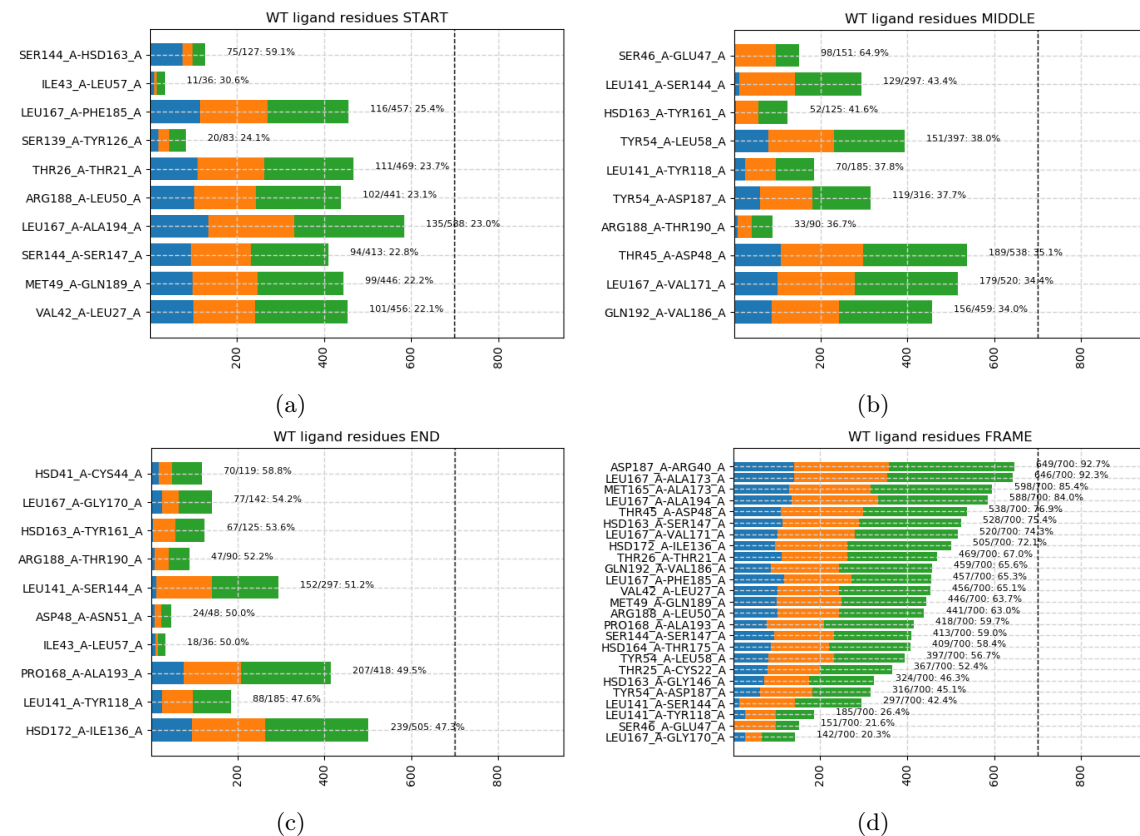


Figure 7: WT protein, bar plots of the interactions involving residues of the **ligand** selection. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered cut-offs of 30% for the "START" section, 40% for the "MIDDLE" section and 50% for the "END" section.

2.4 WT pulling simulation - dimerization

Interactions	Start	Middle	End	Frames
GLY2_A-ASN214_A	30.84%	30.84%	38.32%	107
ARG298_A-VAL303_A	15.69%	19.61%	64.71%	51
GLU290_A-LYS137_A	0.0%	9.62%	90.38%	52

Table 17: WT protein, **dimerization** interactions in the pulling simulation. Sorting method: **Start**.

Interactions	Start	Middle	End	Frames
GLY2_A-ASN214_A	30.84%	30.84%	38.32%	107
GLU290_A-LYS137_A	0.0%	9.62%	90.38%	52
ARG298_A-VAL303_A	15.69%	19.61%	64.71%	51

Table 18: WT protein, **dimerization** interactions in the pulling simulation. Sorting method: **Frames**.

2.4.1 WT protein pulling. Bar plots for the dimerization residues with four sorting methods

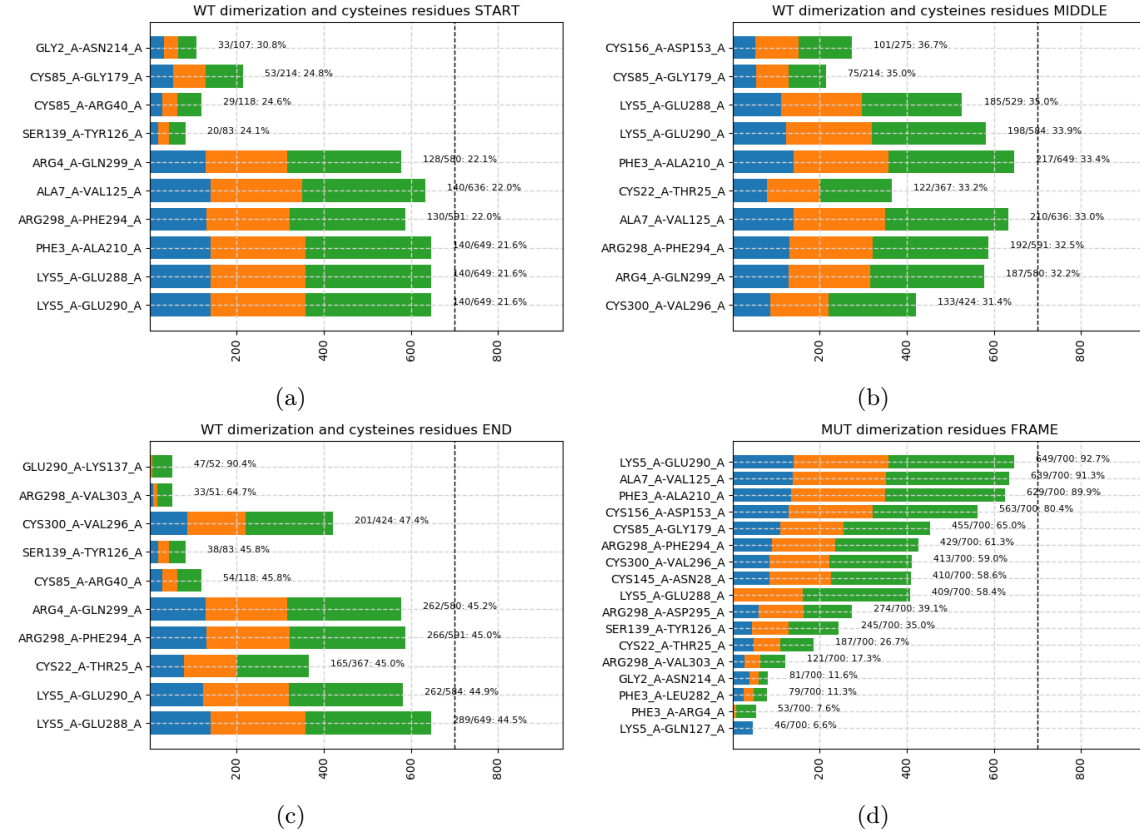


Figure 8: WT protein, bar plots of the interactions involving residues of the **dimerization** selection. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered cut-offs of 30% for the "START" section, 40% for the "MIDDLE" section and 50% for the "END" section.

3 Python packages versions

#	Name	Version	Build	Channel
	libgcc_mutex	0.1	conda_forge	conda-forge
	openmp_mutex	4.5	_2_gnu	conda-forge
	alsa-lib	1.2.8	h166bdaf_0	conda-forge
	anyio	3.5.0	py37h06a4308_0	
	argon2-cffi	21.3.0	pyhd3eb1b0_0	
	argon2-cffi-bindings	21.2.0	py37h7f8727e_0	
	attr	2.5.1	h166bdaf_1	conda-forge
	attrs	20.3.0	pyhd3deb0d_0	conda-forge
	babel	2.11.0	py37h06a4308_0	
	backcall	0.2.0	pyhd3eb1b0_0	
	beautifulsoup4	4.11.1	py37h06a4308_0	
	biopython	1.78	py37h5e8e339_2	conda-forge
	bleach	4.1.0	pyhd3eb1b0_0	
	brotlipy	0.7.0	py37h27cf2d3_1003	
	bzip2	1.0.8	h7f98852_4	conda-forge
	c-ares	1.18.1	h7f98852_0	conda-forge
	ca-certificates	2023.01.10	h06a4308_0	
	cairo	1.16.0	ha61ee94_1014	conda-forge
	certifi	2022.12.7	py37h06a4308_0	
	cffi	1.15.1	py37h5eee18b_3	
	cftime	1.6.1	py37hda87dfa_0	conda-forge
	charset-normalizer	2.0.4	pyhd3eb1b0_0	
	cryptography	38.0.4	py37h9ce1e76_0	
	curl	7.87.0	hdc1c0ab_0	conda-forge
	cycler	0.10.0	py_2	conda-forge
	cython	0.29.23	py37hcd2ae1e_1	conda-forge
	dbus	1.13.6	h5008d03_3	conda-forge
	debugpy	1.5.1	py37h295c915_0	
	decorator	4.4.2	py_0	conda-forge
	defusedxml	0.7.1	pyhd3eb1b0_0	
	entrypoints	0.4	py37h06a4308_0	
	expat	2.5.0	h270877fc_0	conda-forge
	fftw	3.3.10	nompi_hf0379b8_106	conda-forge
	font-ttf-dejavu-sans-mono	2.37	hab24e00_0	conda-forge
	font-ttf-inconsolata	3.000	h77eed37_0	conda-forge
	font-ttf-source-code-pro	2.038	h77eed37_0	conda-forge
	font-ttf-ubuntu	0.83	hab24e00_0	conda-forge
	fontconfig	2.14.1	hc2a2eb6_0	conda-forge
	fonts-conda-ecosystem	1	_0	conda-forge
	fonts-conda-forge	1	_0	conda-forge
	freetype	2.12.1	hca18f0e_1	conda-forge
	fridi	1.0.10	h36c2ea0_0	conda-forge
	gettext	0.21.1	h270877fc_0	conda-forge
	giflib	5.2.1	h36c2ea0_2	conda-forge
	glib	2.74.1	h6239696_1	conda-forge
	glib-tools	2.74.1	h6239696_1	conda-forge
	graphite2	1.3.13	h58526e2_1001	conda-forge
	griddatamats	0.5.0	py_0	conda-forge
	gsd	2.4.2	py37h6f94858_0	conda-forge
	gst-plugins-base	1.21.3	h4243ec0_1	conda-forge
	gstreamer	1.21.3	h25f0c4b_1	conda-forge
	gstreamer	1.21.3	h25f0c4b_1	conda-forge
	gstreamer-orc	0.4.33	h166bdaf_0	conda-forge
	harfbuzz	6.0.0	h8e241bc_0	conda-forge
	hdf4	4.2.15	h9772cbc_5	conda-forge
	hdf5	1.10.5	nompi_h5b725eb_1114	conda-forge
	icu	70.1	h270877fc_0	conda-forge
	idna	3.4	py37h06a4308_0	
	importlib-metadata	4.0.1	py37h89c1867_0	conda-forge
	importlib_metadata	4.0.1	hd8ed1ab_0	conda-forge
	importlib_resources	5.2.0	pyhd3eb1b0_1	
	iniconfig	1.1.1	pyh9f0ad1d_0	conda-forge
	ipykernel	6.15.2	py37h06a4308_0	
	ipython	7.31.1	py37h06a4308_1	
	ipython_genutils	0.2.0	pyhd3eb1b0_1	
	ipywidgets	7.6.5	pyhd3eb1b0_1	
	jack	1.9.21	h583fa2b_2	conda-forge
	jedi	0.18.1	py37h06a4308_1	
	jinja2	3.1.2	py37h06a4308_0	
	jobjlib	1.0.1	pyhd8ed1ab_0	conda-forge
	jpeg	9e	h166bdaf_2	conda-forge
	json5	0.9.6	pyhd3eb1b0_0	
	jsonschema	4.16.0	py37h06a4308_0	
	jupyter	1.0.0	py37h06a4308_8	
	jupyter_client	7.1.2	pyhd3eb1b0_0	
	jupyter_console	6.4.4	py37h06a4308_0	
	jupyter_core	4.11.1	py37h06a4308_0	
	jupyter_server	1.23.4	py37h06a4308_0	
	jupyterlab	3.5.3	py37h06a4308_0	
	jupyterlab_pygments	0.1.2	py_0	
	jupyterlab_server	2.10.3	pyhd3eb1b0_1	
	jupyterlab_widgets	1.0.0	pyhd3eb1b0_1	
	keyutils	1.6.1	h166bdaf_0	conda-forge
	kiwisolver	1.3.1	py37h2527ec5_1	conda-forge
	krb5	1.20.1	h81ceb04_0	conda-forge
	lame	3.100	h166bdaf_1003	conda-forge
	lcms2	2.12	hddcb42_0	conda-forge
	ld_impl_linux-64	2.39	hcc3a1bd_1	conda-forge
	lerc	3.0	h9c3ff4c_0	conda-forge
	libaec	1.0.6	hcb278e6_1	conda-forge
	libblas	3.9.0	16_linux64_openblas	conda-forge
	libcap	2.66	ha37c62d_0	conda-forge
	libcbblas	3.9.0	16_linux64_openblas	conda-forge
	libclang	15.0.7	default_had23c3d_0	conda-forge
	libclang13	15.0.7	default_h3e3d535_0	conda-forge
	libcups	2.3.3	h36d4200_3	conda-forge
	libcurl	7.87.0	hdc1c0ab_0	conda-forge
	libdb	6.2.32	h9c3ff4c_0	conda-forge
	libdeflate	1.10	h7f98852_0	conda-forge
	libedit	3.1.20191231	he28a2e2_2	conda-forge
	libev	4.33	h516909a_1	conda-forge
	libevent	2.1.10	h28343ad_4	conda-forge
	libffi	3.4.2	h7f98852_5	conda-forge
	libflac	1.4.2	h270877fc_0	conda-forge
	libgcc-ng	12.2.0	h65d4601_19	conda-forge
	libgccrypt	1.10.1	h166bdaf_0	conda-forge

libfortran-ng	12.2.0	h69a702a_19	conda-forge	nest-asyncio	1.5.6	py37h06a4308_0		
libfortran5	12.2.0	h337968e_19	conda-forge	netcdf4	1.5.3	nomp1_py37hec16513_103	conda-forge	
libglib	2.74.1	h606061b_1	conda-forge	networkx	2.5.1	pyhd8ed1ab_0		
libgomp	12.2.0	h65d4601_19	conda-forge	notebook	6.5.2	py37h06a4308_0		
libgpg-error	1.46	h620e276_0	conda-forge	notebook-shim	0.2.2	py37h06a4308_0		
libiconv	1.17	h166bdaf_0	conda-forge	nspr	4.35	h27087fc_0	conda-forge	
libimagequant	2.17.0	h7f98852_1	conda-forge	nss	3.02	he02c5a1_0	conda-forge	
liblapack	3.9.0	16_linux64_openblas	conda-forge	numpy	1.20.2	py37h038b26d_0	conda-forge	
liblvm15	15.0.7	hadd5161_0	conda-forge	openjpeg	2.5.0	h7d73246_0	conda-forge	
libnetcdf	4.7.4	nomp1_h9f9fd6a_101	conda-forge	openssl	3.0.7	hb041bf4_2	conda-forge	
libnghttp2	1.51.0	hff17c54_0	conda-forge	packaging	20.9	pyh44b312d_0	conda-forge	
libnsl	2.0.0	h7f98852_0	conda-forge	pandas	1.3.5	py37he8f5f7f_0	conda-forge	
libogg	1.3.4	h7f98852_1	conda-forge	pandocfilters	1.5.0	pyhd3eb1b0_0		
libopenblas	0.3.21	pthreades_h78a6416_3	conda-forge	parso	0.8.3	pyhd3eb1b0_0		
libopus	1.3.1	h7f98852_1	conda-forge	patsy	0.5.3	pyhd8ed1ab_0	conda-forge	
libpng	1.6.39	h753d276_0	conda-forge	pcr2	10.40	hc3806b6_0	conda-forge	
libpq	15.1	hb675445_3	conda-forge	pepext	4.8.0	pyhd3eb1b0_3		
libsndfile	1.2.0	hb75c966_0	conda-forge	pickleshare	0.7.5	pyhd3eb1b0_1003		
libsodium	1.0.18	h7b6447c_0	conda-forge	pillow	9.0.0	py37hc8ad62e_0	conda-forge	
libsqlite	3.40.0	h753d276_0	conda-forge	pip	22.3.1	pyhd8ed1ab_0	conda-forge	
libssh2	1.10.0	hfi4f497_3	conda-forge	pixman	0.40.0	h36c2ea0_0	conda-forge	
libstdcxx-ng	12.2.0	h46fd767_19	conda-forge	pkutil-resolve-name	1.3.10	py37h06a4308_0		
libsystemd0	252	h2a991cd_0	conda-forge	plotly	5.13.0	pypi	pypi	
libtiff	4.3.0	h0fcabac_4	conda-forge	pluggy	0.13.1	py37h89c1867_4	conda-forge	
libtool	2.4.7	h27087fc_0	conda-forge	ply	3.11	py1	conda-forge	
libudev1	252	h166bdaf_0	conda-forge	prometheus-client	0.14.1	py37h06a4308_0		
libuuid	2.32.1	h7f98852_1000	conda-forge	prompt-toolkit	3.0.36	py37h06a4308_0		
libvorbis	1.3.7	h9c3ff4c_0	conda-forge	prompt-toolkit	3.0.36	hd3eb1b0_0		
libwebp	1.2.2	h3452ae3_0	conda-forge	psutil	5.9.0	py37h5ee18b_0		
libwebp-base	1.2.2	h7f98852_1	conda-forge	pthread-stubs	0.4	h36c2ea0_1001	conda-forge	
libxcb	1.13	h7f98852_1004	conda-forge	ptyprocess	0.7.0	pyhd3eb1b0_2		
libxkbcommon	1.0.3	he3ba5ed_0	conda-forge	pulseaudio	16.1	ha8d29e2_1	conda-forge	
libxml2	2.10.3	h7463322_0	conda-forge	py	1.10.0	pyhd3deb0d_0	conda-forge	
libzip	1.9.2	hc929e4a_1	conda-forge	pyparser	2.21	pyhd3eb1b0_0		
libzlib	1.2.13	h166bdaf_4	conda-forge	pygments	2.11.2	pyhd3eb1b0_0		
lz4-c	1.9.3	h9c3ff4c_1	conda-forge	pyinteraph	1.1	pypi	pypi	
markupsafe	2.1.1	py37h7f8727e_0		pyjokes	0.6.0	pyhd3eb1b0_0		
matplotlib	3.3.4	py37h89c1867_0	conda-forge	pyopenssl	22.0.0	pyhd3eb1b0_0		
matplotlib-base	3.3.4	py37h0c9df89_0	conda-forge	pyarsing	3.0.9	pyhd8ed1ab_0	conda-forge	
matplotlib-inline	0.1.6	py37h06a4308_0		pyqt	5.15.7	py37hf30b843_1	conda-forge	
mdanalysis	2.0.0	py37hcd2ae1e_1	conda-forge	pyqt5-sip	12.11.0	py37hd23a5d3_1	conda-forge	
mistune	0.8.4	py37h14c3975_1001		pyrsistent	0.18.0	py37heee7806_0		
mmf-python	1.1.3	pypi	pypi	pysocks	1.7.1	py37_1		
mock	4.0.3	py37h89c1867_3	conda-forge	pytest	6.2.3	py37h89c1867_0	conda-forge	
more-itertools	9.0.0	pyhd8ed1ab_0	conda-forge	python	3.7.12	hf930737_100_cpython	conda-forge	
mpg123	1.31.2	hcb278e6_0	conda-forge	python-dateutil	2.8.1	py	conda-forge	
msgpack-python	1.0.4	py37h7cecd7_0	conda-forge	python-fastjsonschema	2.16.2	py37h06a4308_0		
mysql-common	8.0.32	ha901b37_0	conda-forge	python_abi	3.7	3_cp37m	conda-forge	
mysql-libs	8.0.32	hd7da12d_0	conda-forge	pytz	2021.1	pyhd8ed1ab_0	conda-forge	
nbclassic	0.4.8	py37h06a4308_0		pyzmq	23.2.0	py37h6a678d5_0		
nbclient	0.5.13	py37h06a4308_0		qt-main	5.15.6	he02db52_6	conda-forge	
nbconvert	6.4.4	py37h06a4308_0		qtconsole	5.4.0	py37h06a4308_0		
nbformat	5.7.0	py37h06a4308_0		qtpy	2.2.0	py37h06a4308_0		
ncurses	6.3	h27087fc_1	conda-forge	readline	8.1.2	h0f457ee_0	conda-forge	

readline	8.1.2	h8f457ee_0	conda-forge
requests	2.28.1	py37h06a4308_0	
scikit-learn	1.0.2	py37hf9e9bfc_0	conda-forge
scipy	1.7.3	py37hf2a6cf1_0	conda-forge
seaborn	0.11.1	hd8ed1ab_1	conda-forge
seaborn-base	0.11.1	pyhd8ed1ab_1	conda-forge
send2trash	1.8.0	pyhd3eb1b0_1	
setuptools	59.8.0	py37h89c1867_1	conda-forge
sip	6.7.2	py37hd23a5d3_0	conda-forge
six	1.15.0	pyh9f0ad1d_0	conda-forge
sniffio	1.2.0	py37h06a4308_1	
soupsieve	2.3.2.post1	py37h06a4308_0	
sqlite	3.40.0	h4ff8645_0	conda-forge
statsmodels	0.13.2	py37hda87dfa_0	conda-forge
tenacity	8.1.0	pypi_0	pypi
terminado	0.17.1	py37h06a4308_0	
testpath	0.6.0	py37h06a4308_0	
threadpoolctl	3.1.0	pyh8a188c0_0	conda-forge
tk	8.6.12	h27826a3_0	conda-forge
toml	0.10.2	pyhd8ed1ab_0	conda-forge
tomli	2.0.1	py37h06a4308_0	
tornado	6.2	py37h540881e_0	conda-forge
tqdm	4.60.0	pyhd8ed1ab_0	conda-forge
traitlets	5.7.1	py37h06a4308_0	
typing-extensions	3.7.4.3	0	conda-forge
typing_extensions	3.7.4.3	py_0	conda-forge
urllib3	1.26.14	py37h06a4308_0	
vmd-python	3.0.6	py37h1c6463b_5	conda-forge
wcwidth	0.2.5	pyhd3eb1b0_0	
webencodings	0.5.1	py37_1	
websocket-client	0.58.0	py37h06a4308_4	
wheel	0.38.4	pyhd8ed1ab_0	conda-forge
widgetsnbextension	3.5.2	py37h06a4308_0	
xcb-util	0.4.0	h166bdaf_0	conda-forge
xcb-util-image	0.4.0	h166bdaf_0	conda-forge
xcb-util-keysyms	0.4.0	h166bdaf_0	conda-forge
xcb-util-renderutil	0.3.9	h166bdaf_0	conda-forge
xcb-util-wm	0.4.1	h166bdaf_0	conda-forge
xorg-kbproto	1.0.7	h7f98852_1002	conda-forge
xorg-libice	1.0.10	h7f98852_0	conda-forge
xorg-libsm	1.2.3	hd9c2040_1000	conda-forge
xorg-libx11	1.7.2	h7f98852_0	conda-forge
xorg-libxau	1.0.9	h7f98852_0	conda-forge
xorg-libxdmcp	1.1.3	h7f98852_0	conda-forge
xorg-libxext	1.3.4	h7f98852_1	conda-forge
xorg-libxrender	0.9.10	h7f98852_1003	conda-forge
xorg-renderproto	0.11.1	h7f98852_1002	conda-forge
xorg-xextproto	7.3.0	h7f98852_1002	conda-forge
xorg-xproto	7.0.31	h7f98852_1007	conda-forge
xz	5.2.6	h166bdaf_0	conda-forge
zeromq	4.3.4	h2531618_0	
zipp	3.4.1	pyhd8ed1ab_0	conda-forge
zlib	1.2.13	h166bdaf_4	conda-forge
zstd	1.5.2	h3eb15da_6	conda-forge