Supplementary file

Contents

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 Åwere 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
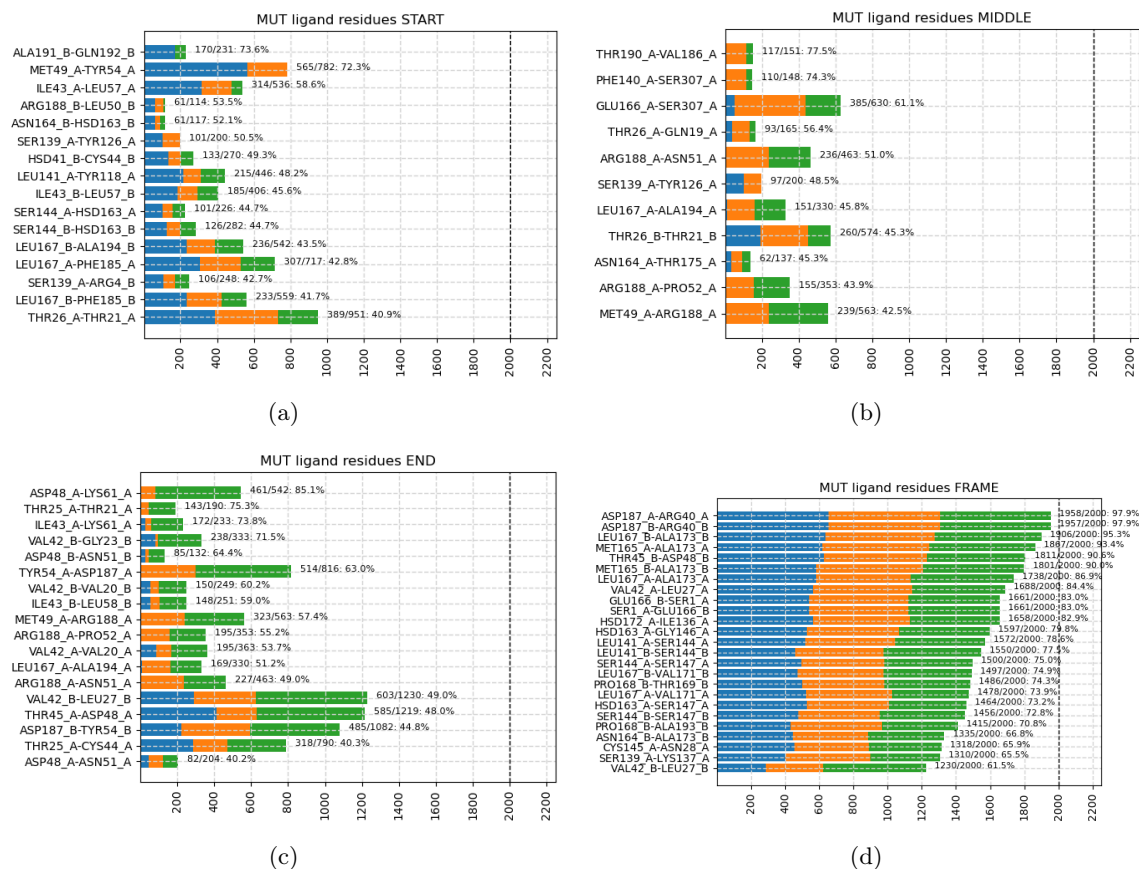

Figure 1: MUT protein, bar plots of the interactions involving residues interacting with the ligand. Each graph lists the interactions with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). We estimated a cut-off of 40% to consider an interaction particularly present in a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

(a)

(b)

(c)

(d)

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
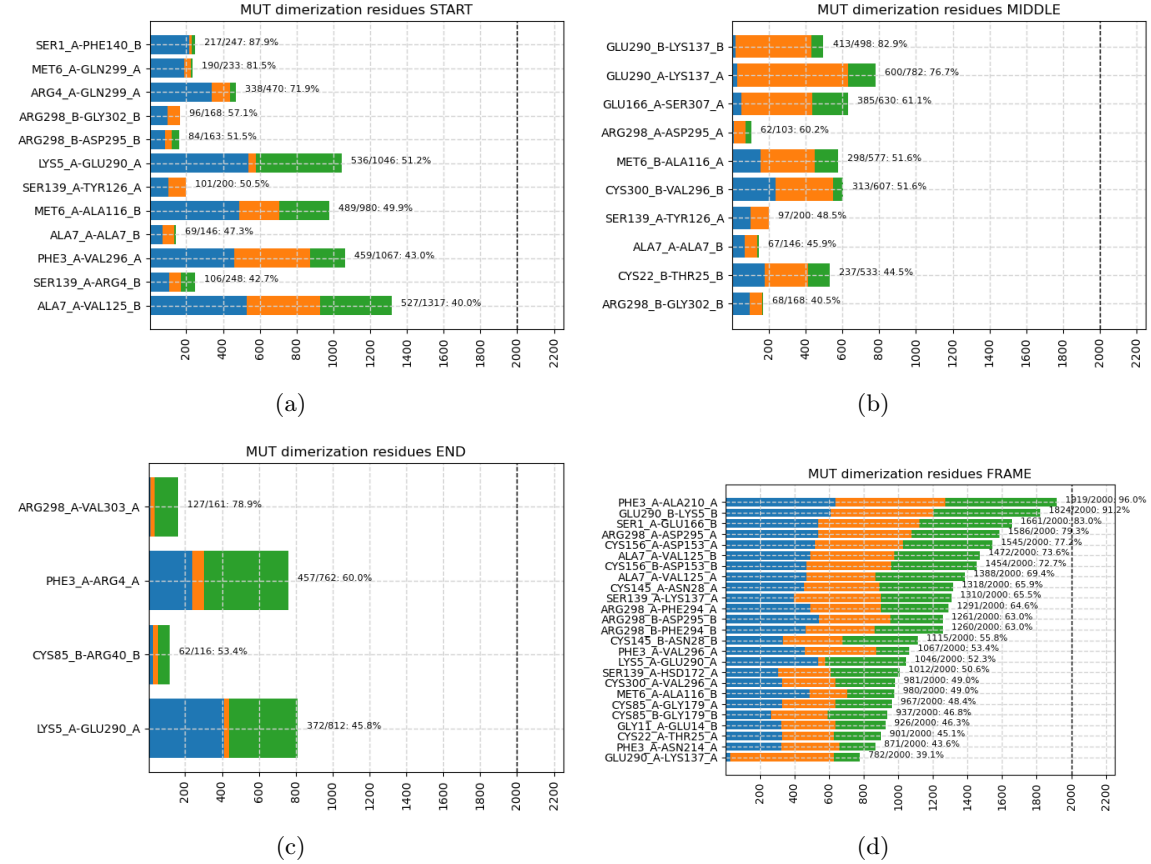

(a)

(b)

(c)

(d)

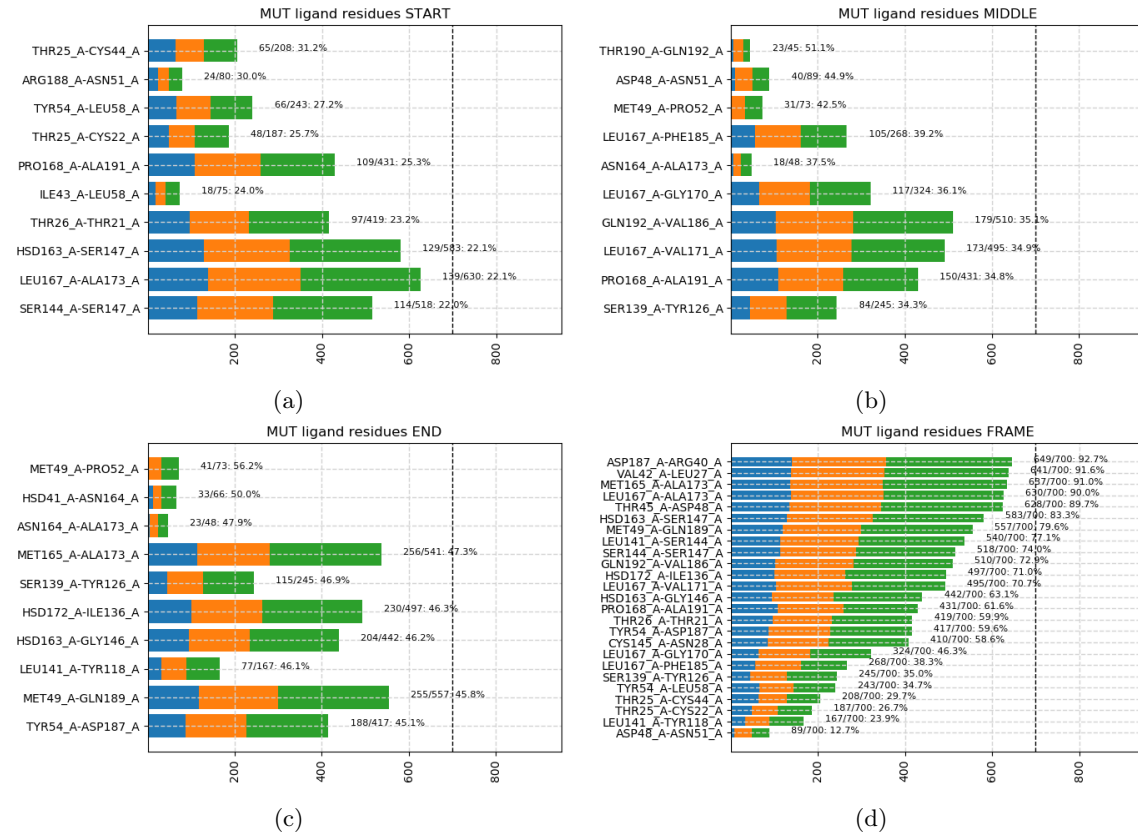Figure 3: MUT protein, bar plots of the interactions involving residues of the **Ligand** residues. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered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

9

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

(a)

(b)

(c)

(d)

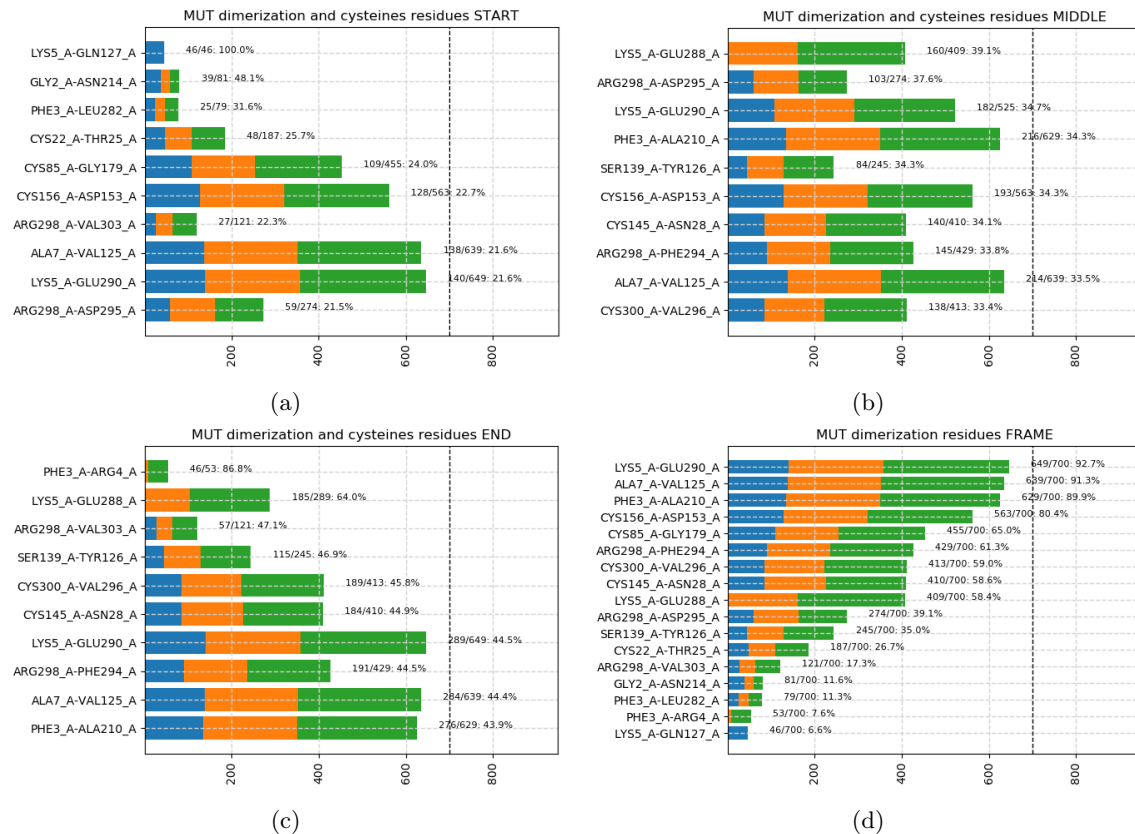Figure 4: MUT protein, bar plots of the interactions involving residues of the **Dimerization** selection. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered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

(a)

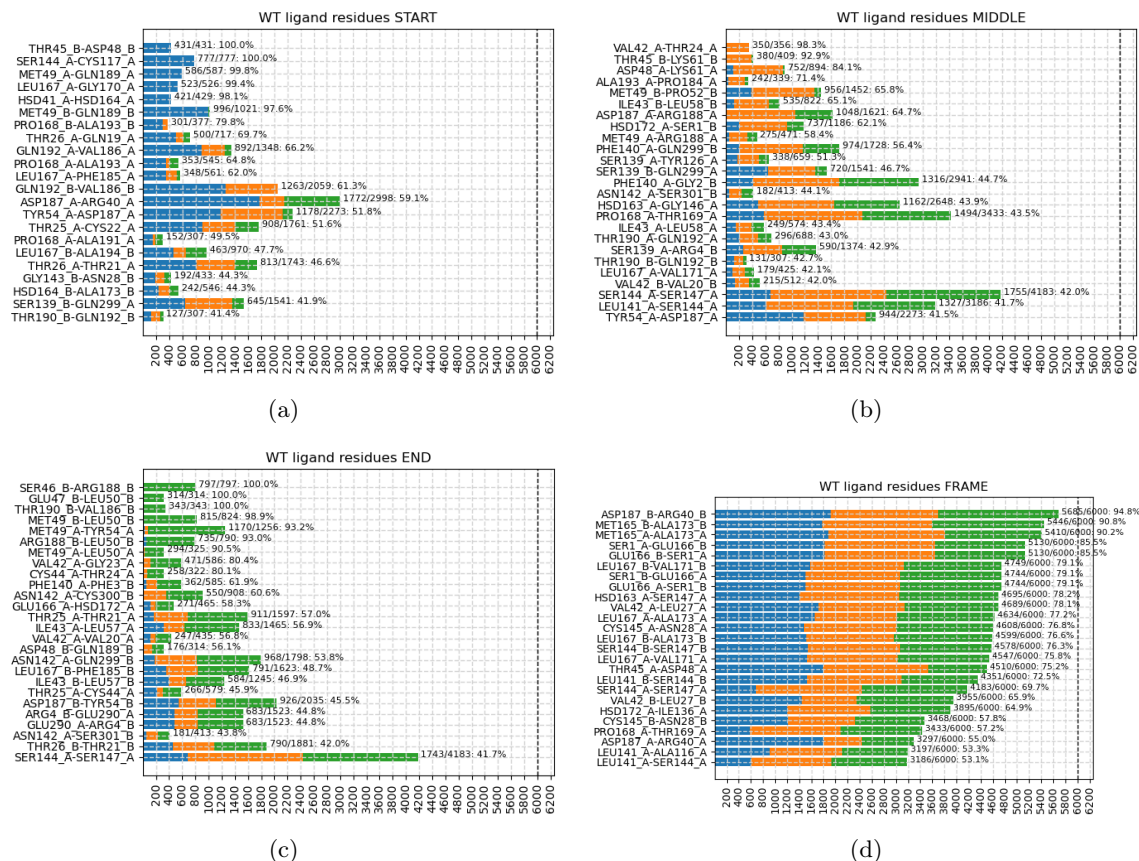(b)

(c)

(d)

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.

16

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**.

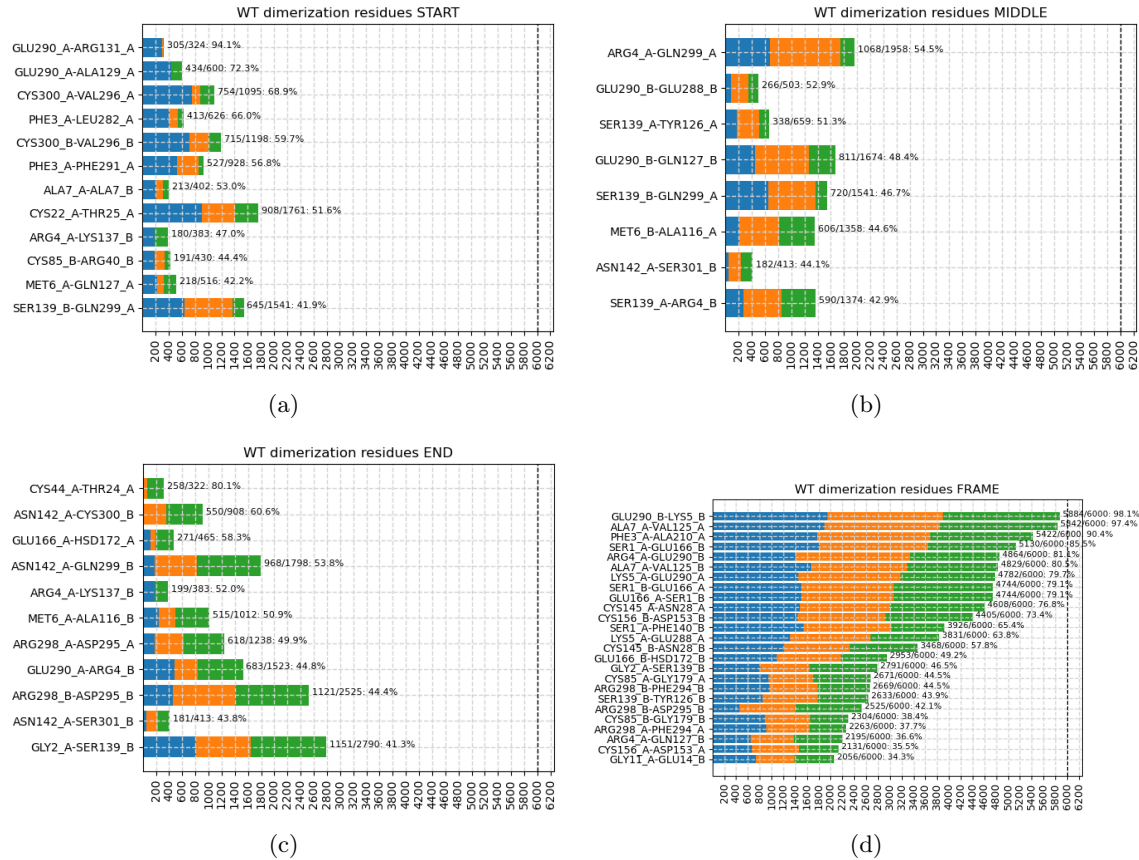## 2.2.1 WT protein: bar plots for the dimerization residues with four sorting methods

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

(a)

(b)

(c)

(d)

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
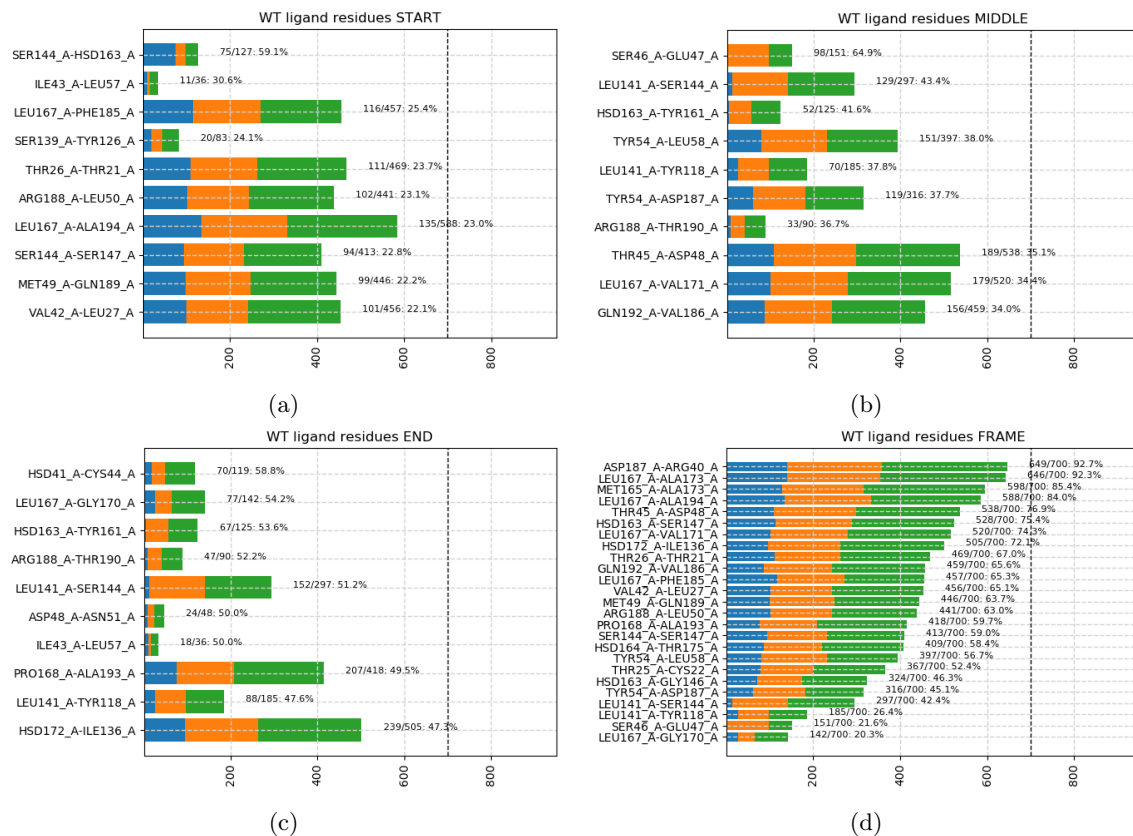

(a)

(b)

(c)

(d)

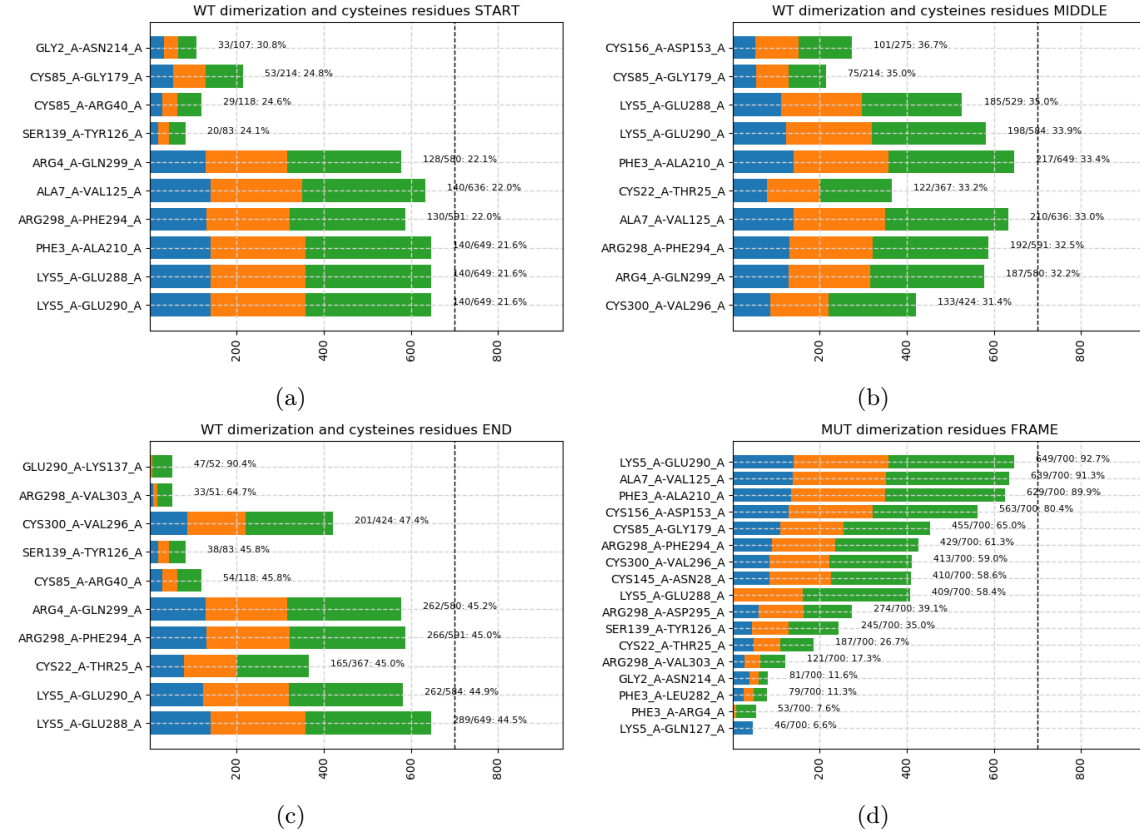Figure 8: WT protein, bar plots of the interactions involving residues of the **dimerization** selection. Each graph lists with the highest appearance rate in a specific fragment ("START", "MIDDLE", "END"). Finally, the figure in the bottom right corner represents the most present interactions. We considered 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	py37h27cfd23_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	
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	h27087fc_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
fribidi	1.0.10	h36c2ea0_0	conda-forge
gettext	0.21.1	h27087fc_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
griddataformats	0.5.0	py_0	
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-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	h27087fc_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	
joblib	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	hddcbb42_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
libcblas	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	h27087fc_0	conda-forge
libgcc-ng	12.2.0	h65d4601_19	conda-forge
libgcrypt	1.10.1	h166bdaf_0	conda-forge

Package	Version	Build	Channel
libgfortran-ng	12.2.0	h69a702a_19	conda-forge
libgfortran5	12.2.0	h337968e_19	conda-forge
libglib	2.74.1	h606061b_1	conda-forge
libgomp	12.2.0	h65d4601_19	conda-forge
libgpg-error	1.46	h620e276_0	conda-forge
libiconv	1.17	h166bdaf_0	conda-forge
libimagequant	2.17.0	h7f98852_1	conda-forge
liblapack	3.9.0	16_linux64_openblas	conda-forge
libllvm15	15.0.7	hadd5161_0	conda-forge
libnetcdf	4.7.4	nompi_h9f9fd6a_101	conda-forge
libnghttp2	1.51.0	hff17c54_0	conda-forge
libnsl	2.0.0	h7f98852_0	conda-forge
libogg	1.3.4	h7f98852_1	conda-forge
libopenblas	0.3.21	pthreads_h78a6416_3	conda-forge
libopus	1.3.1	h7f98852_1	conda-forge
libpng	1.6.39	h753d276_0	conda-forge
libpq	15.1	hb675445_3	conda-forge
libsndfile	1.2.0	hb75c966_0	conda-forge
libsodium	1.0.18	h7b6447c_0	
libsqlite	3.40.0	h753d276_0	conda-forge
libssh2	1.10.0	hf14f497_3	conda-forge
libstdcxx-ng	12.2.0	h46fd767_19	conda-forge
libsystemd0	252	h2a991cd_0	conda-forge
libtiff	4.3.0	h0fcbabc_4	conda-forge
libtool	2.4.7	h27087fc_0	conda-forge
libudev1	252	h166bdaf_0	conda-forge
libuuid	2.32.1	h7f98852_1000	conda-forge
libvorbis	1.3.7	h9c3ff4c_0	conda-forge
libwebp	1.2.2	h3452ae3_0	conda-forge
libwebp-base	1.2.2	h7f98852_1	conda-forge
libxcb	1.13	h7f98852_1004	conda-forge
libxkbcommon	1.0.3	he3ba5ed_0	conda-forge
libxml2	2.10.3	h7463322_0	conda-forge
libzip	1.9.2	hc929e4a_1	conda-forge
libzlib	1.2.13	h166bdaf_4	conda-forge
lz4-c	1.9.3	h9c3ff4c_1	conda-forge
markupsafe	2.1.1	py37h7f8727e_0	
matplotlib	3.3.4	py37h89c1867_0	conda-forge
matplotlib-base	3.3.4	py37h0c9df89_0	conda-forge
matplotlib-inline	0.1.6	py37h06a4308_0	
mdanalysis	2.0.0	py37hcd2ae1e_1	conda-forge
mistune	0.8.4	py37h14c3975_1001	
mmtf-python	1.1.3	pypi_0	pypi
mock	4.0.3	py37h89c1867_3	conda-forge
more-itertools	9.0.0	pyhd8ed1ab_0	conda-forge
mpg123	1.31.2	hcb278e6_0	conda-forge
msgpack-python	1.0.4	py37h7cecad7_0	conda-forge
mysql-common	8.0.32	ha901b37_0	conda-forge
mysql-libs	8.0.32	hd7da12d_0	conda-forge
nbclassic	0.4.8	py37h06a4308_0	
nbclient	0.5.13	py37h06a4308_0	
nbconvert	6.4.4	py37h06a4308_0	
nbformat	5.7.0	py37h06a4308_0	
ncurses	6.3	h27087fc_1	conda-forge

Package	Version	Build	Channel
nest-asyncio	1.5.6	py37h06a4308_0	
netcdf4	1.5.3	nompi_py37hec16513_103	conda-forge
networkx	2.5.1	pyhd8ed1ab_0	conda-forge
notebook	6.5.2	py37h06a4308_0	
notebook-shim	0.2.2	py37h06a4308_0	
nspr	4.35	h27087fc_0	conda-forge
nss	3.82	he02c5a1_0	conda-forge
numpy	1.20.2	py37h038b26d_0	conda-forge
openjpeg	2.5.0	h7d73246_0	conda-forge
openssl	3.0.7	h0b41bf4_2	conda-forge
packaging	20.9	pyh44b312d_0	conda-forge
pandas	1.3.5	py37he8f5f7f_0	conda-forge
pandocfilters	1.5.0	pyhd3eb1b0_0	
parso	0.8.3	pyhd3eb1b0_0	
patsy	0.5.3	pyhd8ed1ab_0	conda-forge
pcre2	10.40	hc3806b6_0	conda-forge
pexpect	4.8.0	pyhd3eb1b0_3	
pickleshare	0.7.5	pyhd3eb1b0_1003	
pillow	9.0.0	py37hc8ad62e_0	conda-forge
pip	22.3.1	pyhd8ed1ab_0	conda-forge
pixman	0.40.0	h36c2ea0_0	conda-forge
pkgutil-resolve-name	1.3.10	py37h06a4308_0	
plotly	5.13.0	pypi_0	pypi
pluggy	0.13.1	py37h89c1867_4	conda-forge
ply	3.11	py_1	conda-forge
prometheus_client	0.14.1	py37h06a4308_0	
prompt-toolkit	3.0.36	py37h06a4308_0	
prompt_toolkit	3.0.36	hd3eb1b0_0	
psutil	5.9.0	py37h5eee18b_0	
pthread-stubs	0.4	h36c2ea0_1001	conda-forge
ptyprocess	0.7.0	pyhd3eb1b0_2	
pulseaudio	16.1	ha8d29e2_1	conda-forge
py	1.10.0	pyhd3deb0d_0	conda-forge
pycparser	2.21	pyhd3eb1b0_0	
pygments	2.11.2	pyhd3eb1b0_0	
pyinteraph	1.1	pypi_0	pypi
pyjokes	0.6.0	pypi_0	pypi
pyopenssl	22.0.0	pyhd3eb1b0_0	
pyparsing	3.0.9	pyhd8ed1ab_0	conda-forge
pyqt	5.15.7	py37hf30b843_1	conda-forge
pyqt5-sip	12.11.0	py37hd23a5d3_1	conda-forge
pyrsistent	0.18.0	py37heee7806_0	
pysocks	1.7.1	py37_1	
pytest	6.2.3	py37h89c1867_0	conda-forge
python	3.7.12	hf930737_100_cpython	conda-forge
python-dateutil	2.8.1	py_0	conda-forge
python-fastjsonschema	2.16.2	py37h06a4308_0	
python_abi	3.7	3_cp37m	conda-forge
pytz	2021.1	pyhd8ed1ab_0	conda-forge
pyzmq	23.2.0	py37h6a678d5_0	
qt-main	5.15.6	h602db52_6	conda-forge
qtconsole	5.4.0	py37h06a4308_0	
qtpy	2.2.0	py37h06a4308_0	
readline	8.1.2	h0f457ee_0	conda-forge

```
readline                8.1.2                      h0f457ee_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
```