Energy Minimization

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Universidade Federal do Rio Grande do Sul

Bioinformática Estrutural, 2017

Roteiro

Solução de Problemas

- Montagem
- 1L2Y

Builder

Builder

Montagem

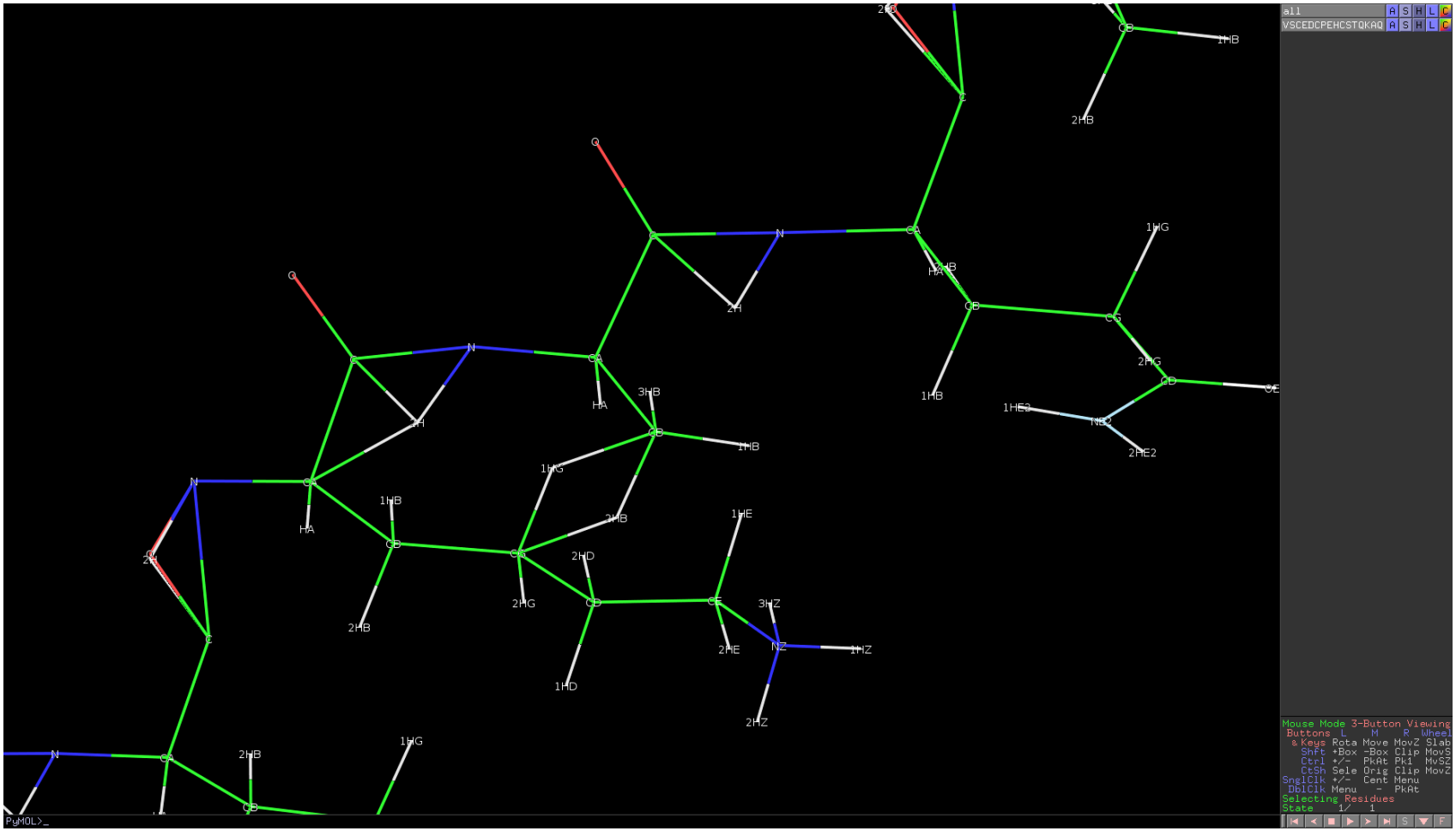


Figura: Ligação tripla de hidrogenios e ângulo de ligação

Solução

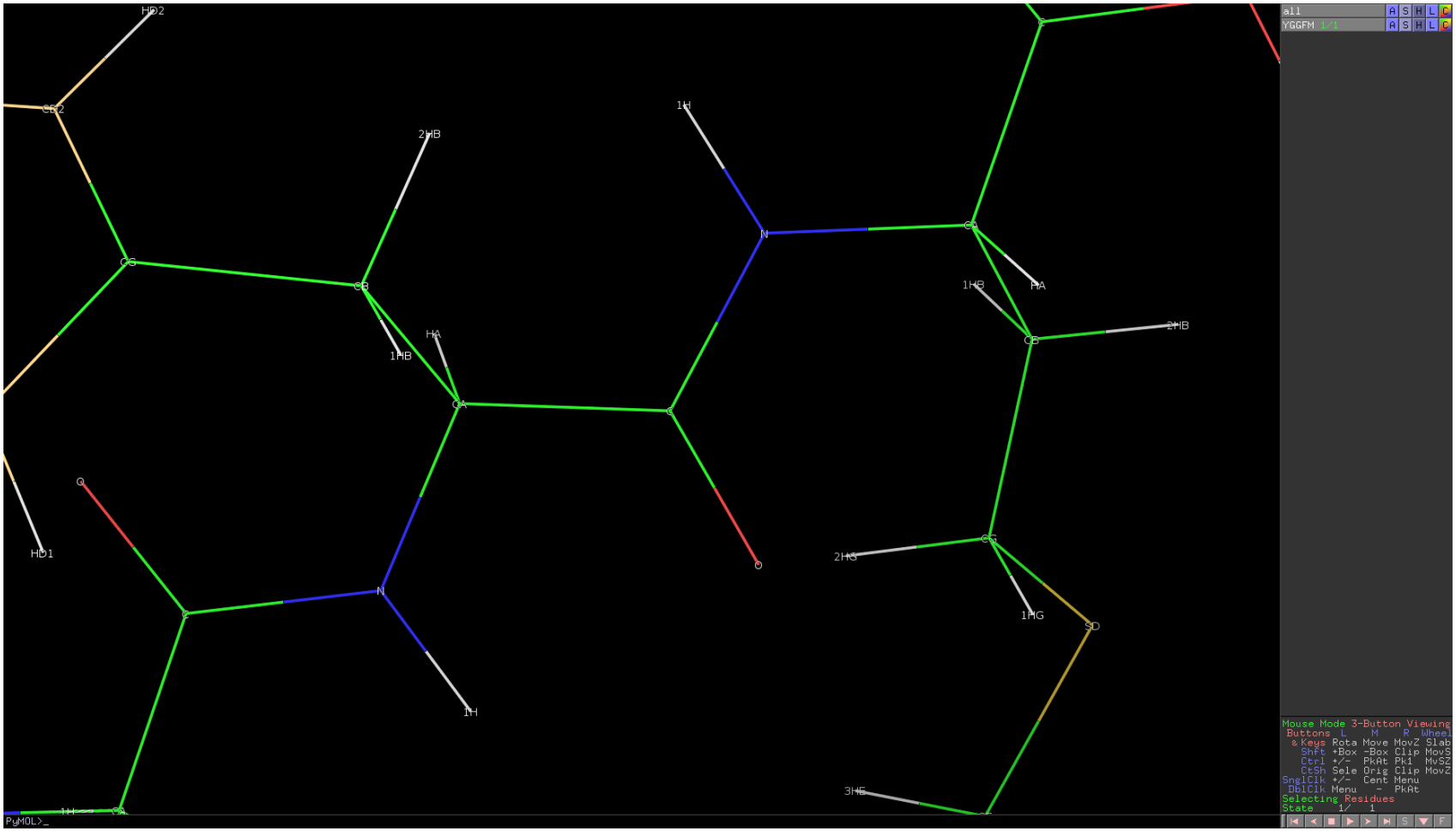


Figura: Ligação tripla de hidrogenios e ângulo de ligação

Rotação de ângulos:

- Não deve modificar a posição

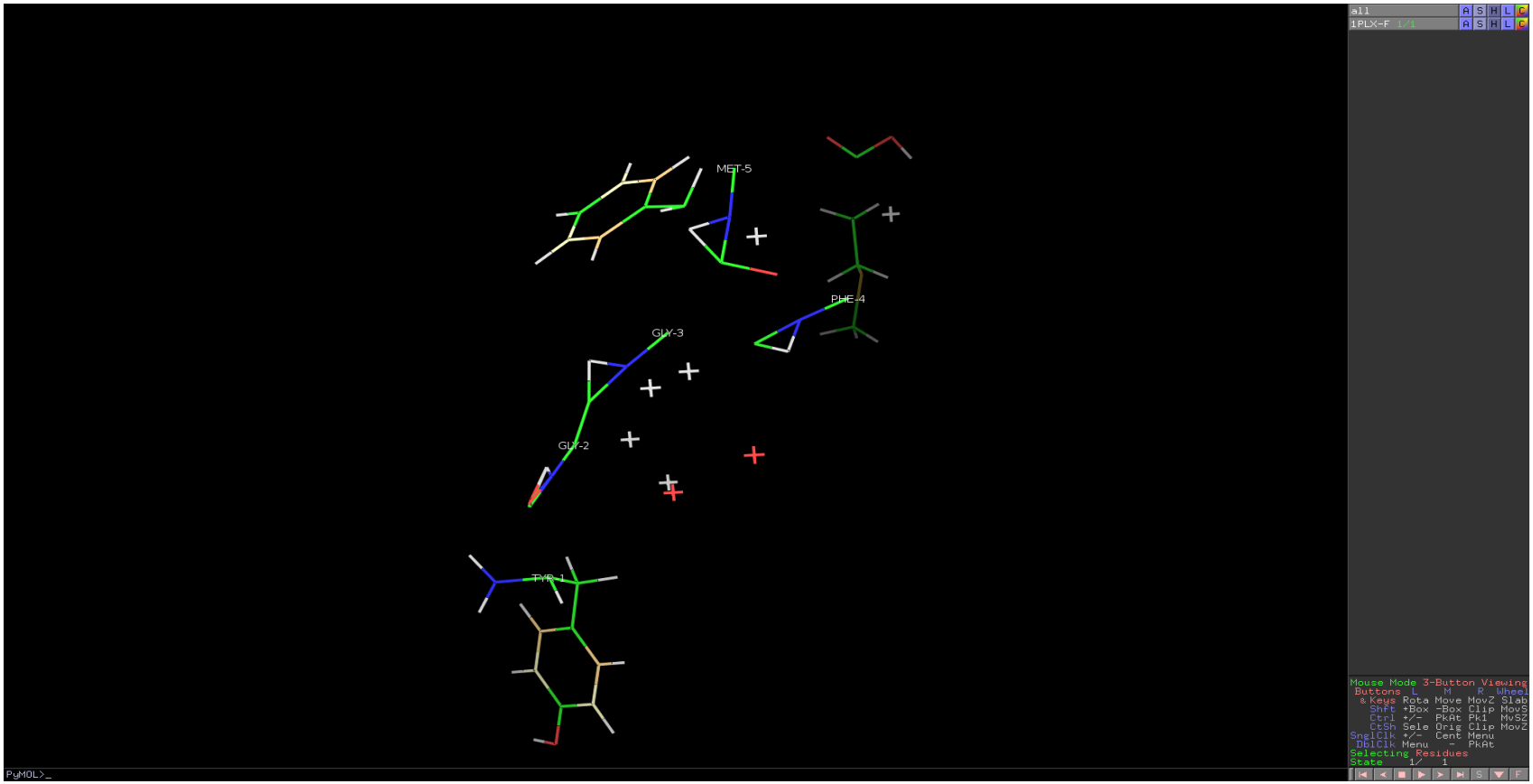


Figura: Resíduos fragmentados por uma rotação errada

Rotação de ângulos:

- Simulated Annealig:

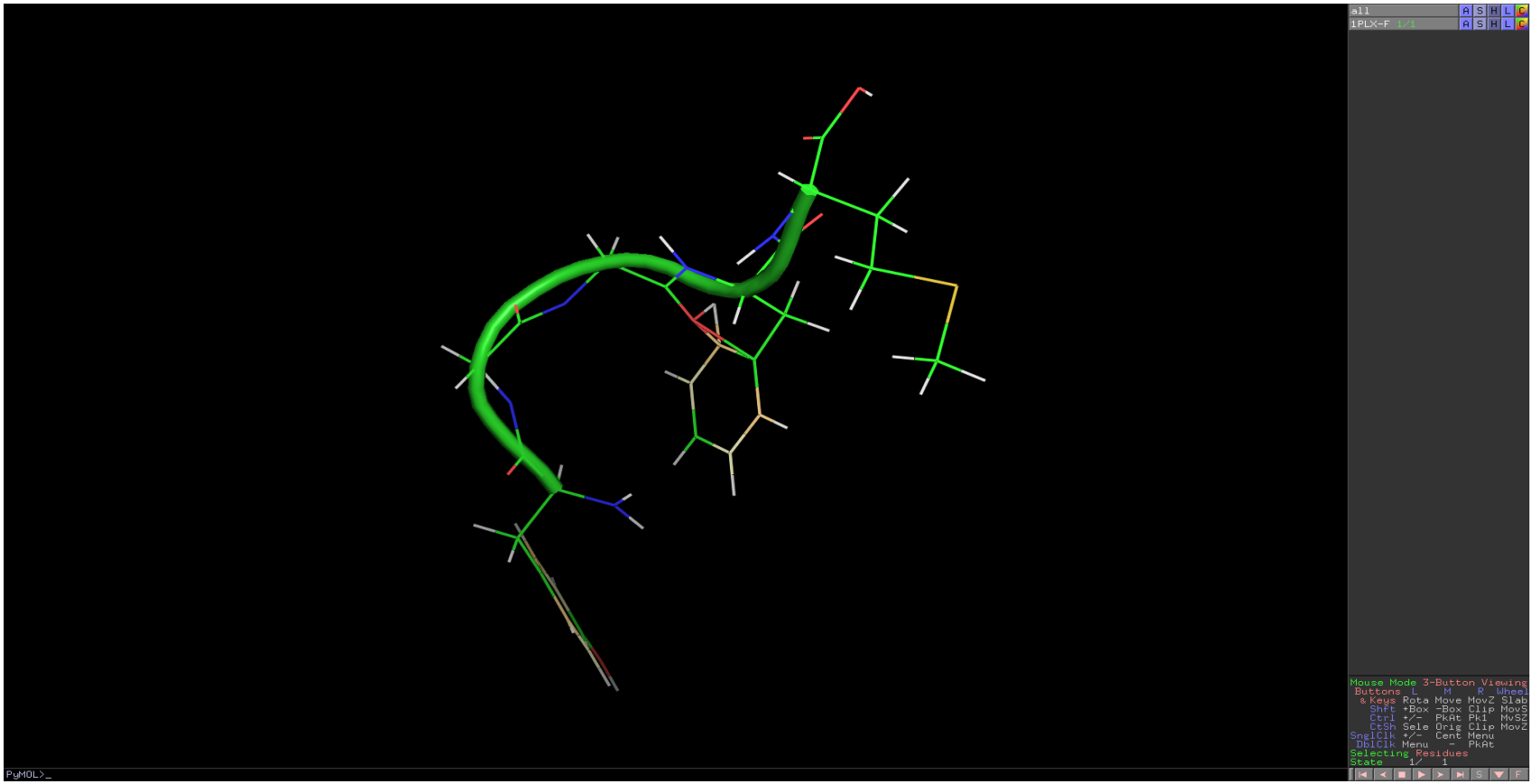
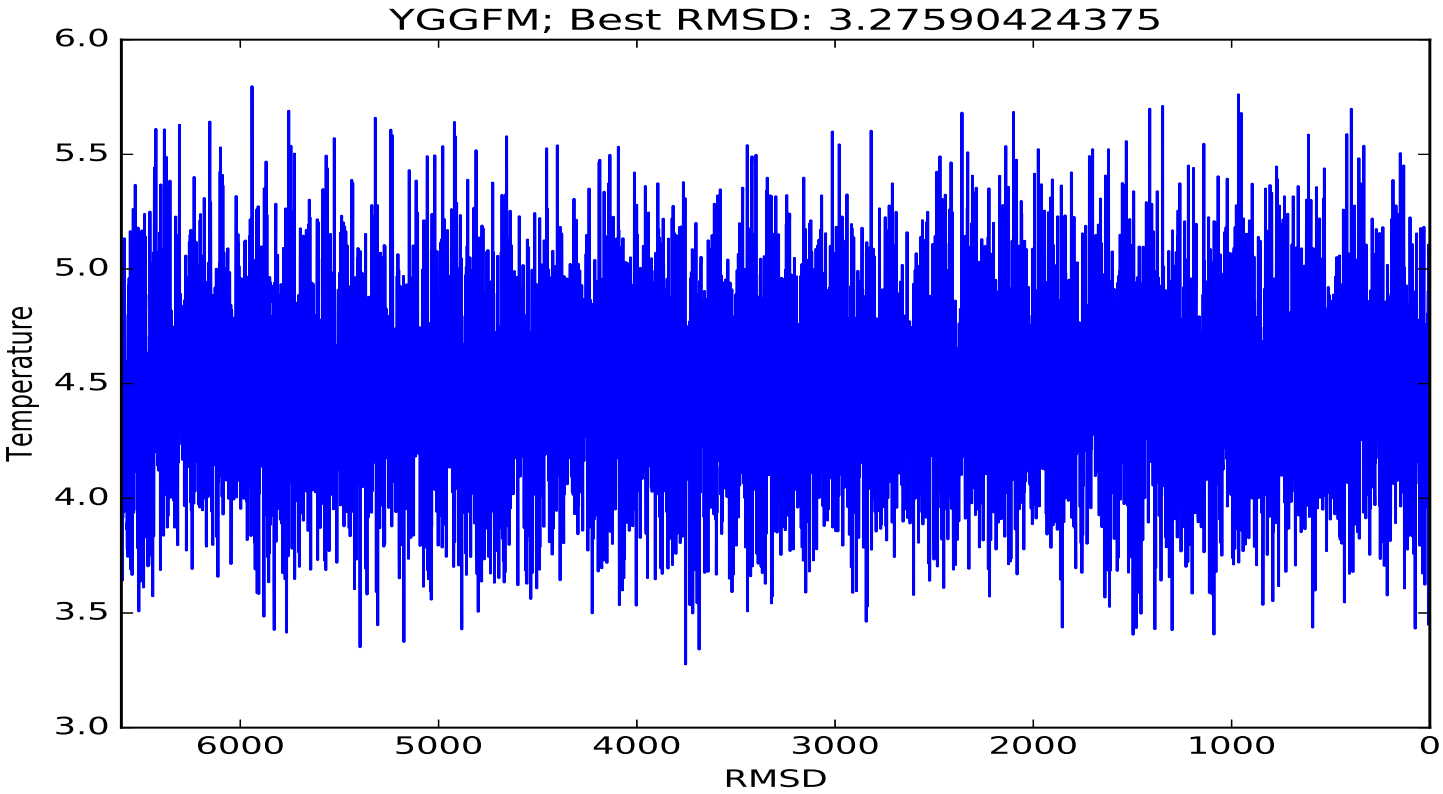


Figura: Resíduos rotacionados através do cálculo de menor RMSD

Rotação de ângulos:

- Simulated Annealig:



Rotação de ângulos:

- Simulated Annealig:

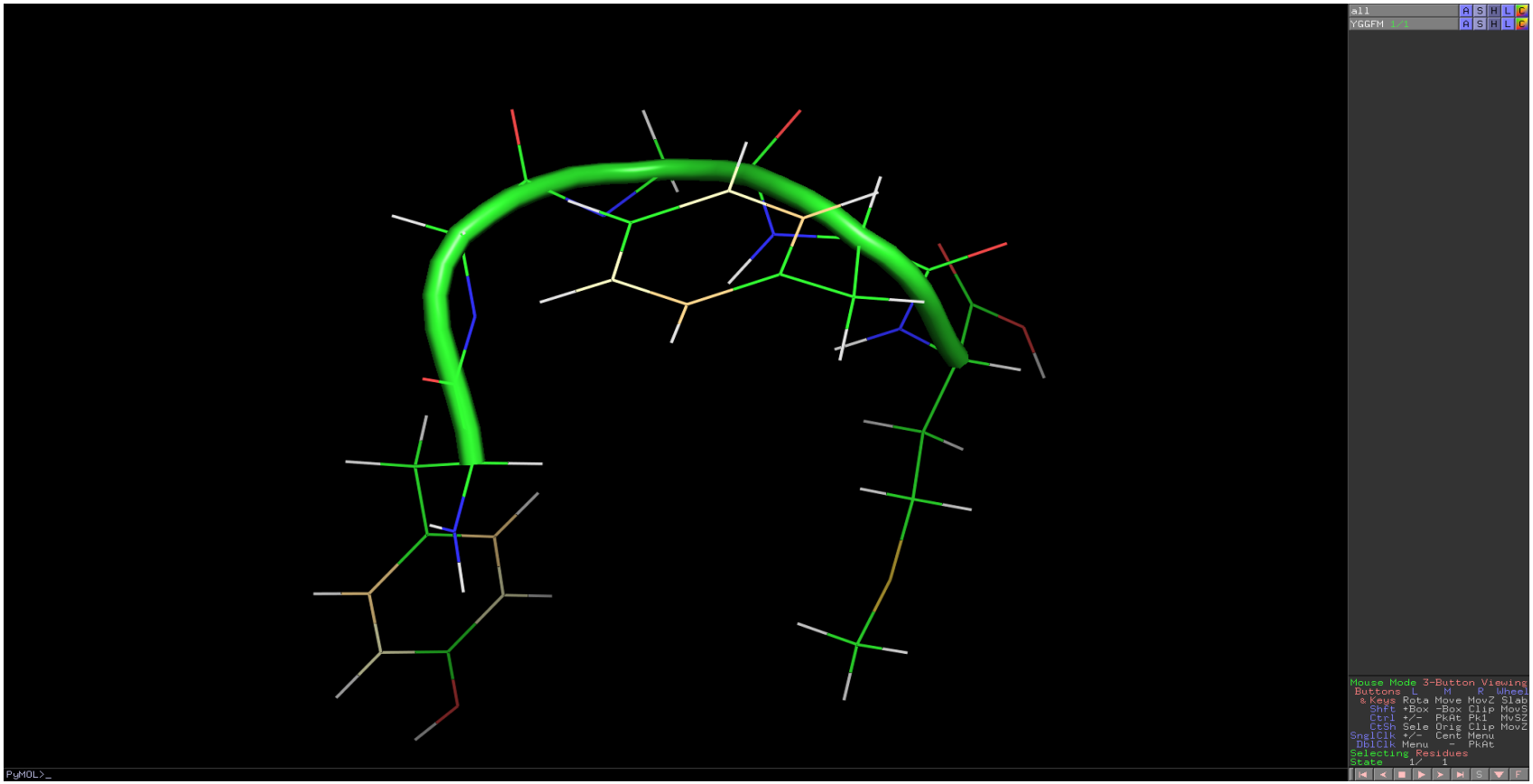


Figura: Resíduos rotacionados com valores de PHI e PSI corretos

Rotação de ângulos:

- Simulated Annealig:

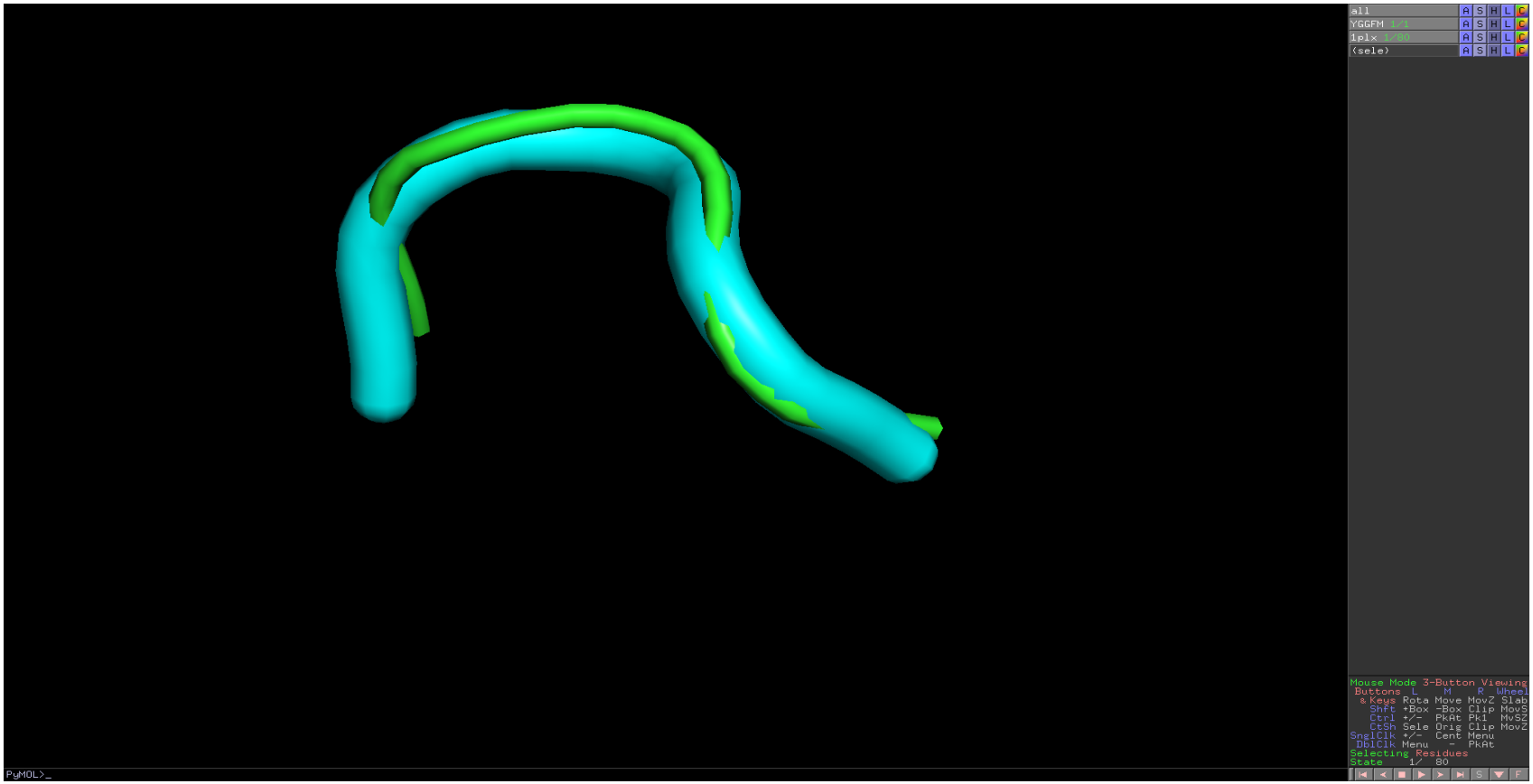


Figura: Sobreposição do YGGFM.pdb e 1PLX.pdb

Rotação de ângulos:

- Simulated Annealig:

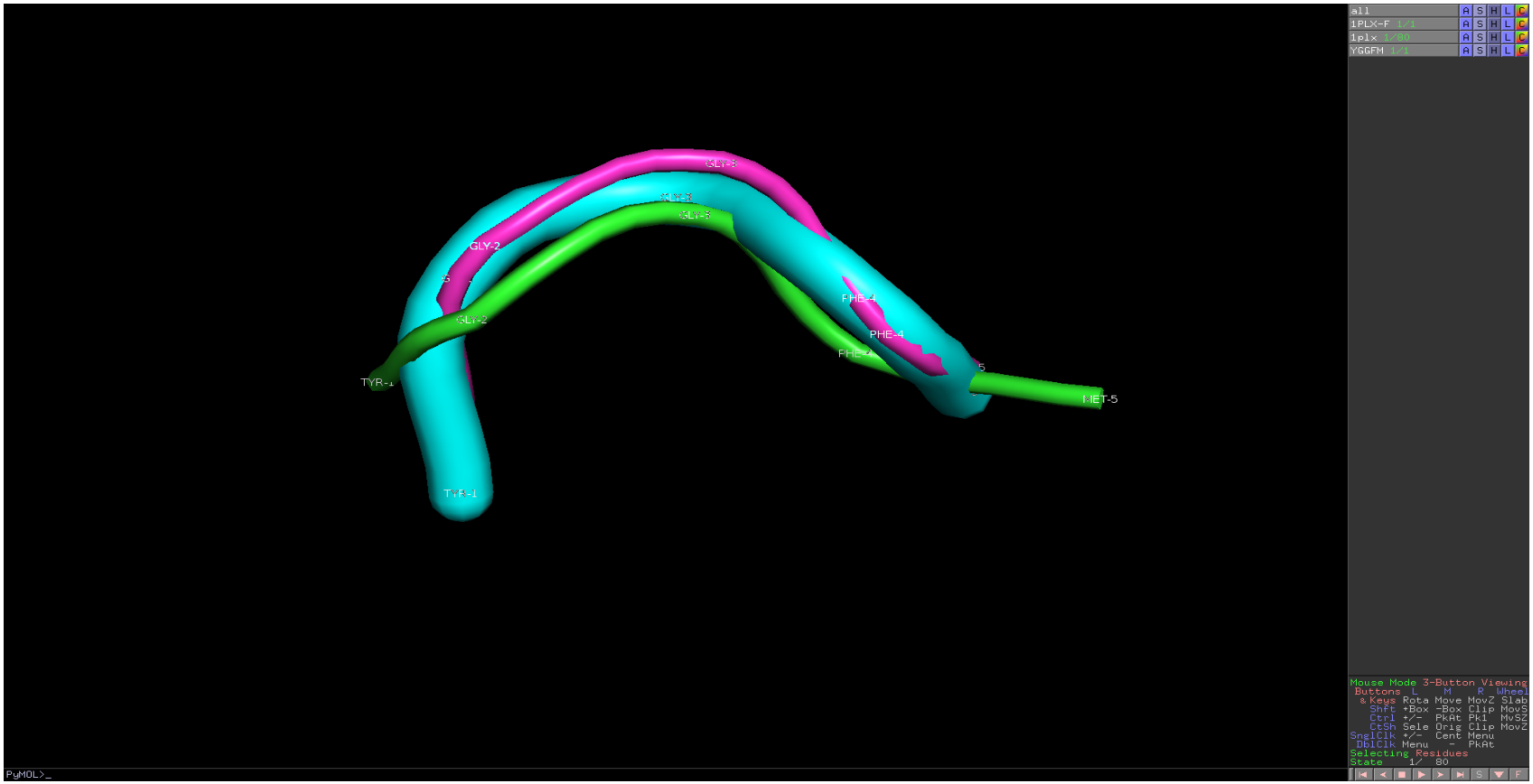


Figura: Sobreposição das 3 estruturas

Arquivo PDB:

- Antigo:

1	ATOM	1	N	VAL	1	0.095	-0.181	0.000	1.00	0.00
2	ATOM	2	CA	VAL	1	1.547	-0.026	0.000	1.00	0.00
3	ATOM	3	C	VAL	1	1.935	1.434	0.000	1.00	0.00
4	ATOM	4	O	VAL	1	1.090	2.337	0.000	1.00	0.00
5	ATOM	5	CB	VAL	1	2.166	-0.772	-1.248	1.00	0.00
6	ATOM	6	CG1	VAL	1	1.977	-2.308	-1.217	1.00	0.00
7	ATOM	7	CG2	VAL	1	3.683	-0.551	-1.501	1.00	0.00
8	ATOM	8	1H	VAL	1	-0.571	0.669	0.000	1.00	0.00
9	ATOM	9	2H	VAL	1	-0.377	-1.152	0.000	1.00	0.00
10	ATOM	10	HA	VAL	1	1.952	-0.468	0.928	1.00	0.00
11	ATOM	11	HB	VAL	1	1.638	-0.395	-2.150	1.00	0.00
12	ATOM	12	1HG1	VAL	1	2.529	-2.782	-0.384	1.00	0.00
13	ATOM	13	2HG1	VAL	1	0.914	-2.590	-1.107	1.00	0.00
14	ATOM	14	3HG1	VAL	1	2.323	-2.783	-2.155	1.00	0.00
15	ATOM	15	1HG2	VAL	1	4.307	-0.876	-0.647	1.00	0.00
16	ATOM	16	2HG2	VAL	1	4.043	-1.094	-2.396	1.00	0.00
17	ATOM	17	3HG2	VAL	1	3.928	0.511	-1.696	1.00	0.00
18	ATOM	18	N	SER	2	3.338	1.708	0.000	1.00	0.00
19	ATOM	19	CA	SER	2	4.797	1.744	0.000	1.00	0.00
20	ATOM	20	C	SER	2	5.304	3.166	0.000	1.00	0.00
21	ATOM	21	O	SER	2	4.539	4.131	0.000	1.00	0.00
22	ATOM	22	CB	SER	2	5.368	0.935	-1.192	1.00	0.00
23	ATOM	23	OG	SER	2	5.119	1.557	-2.457	1.00	0.00
24	ATOM	24	2H	SER	2	2.788	0.778	0.000	1.00	0.00
25	ATOM	25	HA	SER	2	5.149	1.278	0.939	1.00	0.00
26	ATOM	26	1HB	SER	2	6.463	0.817	-1.072	1.00	0.00
27	ATOM	27	2HB	SER	2	4.970	-0.098	-1.203	1.00	0.00
28	ATOM	28	HG	SER	2	4.166	1.586	-2.580	1.00	0.00
29	ATOM	29	N	CYS	3	6.725	3.326	0.000	1.00	0.00
30	ATOM	30	CA	CYS	3	8.181	3.440	0.000	1.00	0.00
31	ATOM	31	C	CYS	3	8.609	4.888	0.000	1.00	0.00
32	ATOM	32	O	CYS	3	7.788	5.817	0.000	1.00	0.00
33	ATOM	33	CB	CYS	3	8.734	2.662	-1.210	1.00	0.00
34	ATOM	34	SG	CYS	3	10.539	2.613	-1.168	1.00	0.00
35	ATOM	35	2H	CYS	3	6.226	2.368	0.000	1.00	0.00
36	ATOM	36	HA	CYS	3	8.565	2.984	0.931	1.00	0.00
37	ATOM	37	1HB	CYS	3	8.366	1.620	-1.218	1.00	0.00
38	ATOM	38	2HB	CYS	3	8.401	3.112	-2.168	1.00	0.00
39	ATOM	39	HG	CYS	3	10.746	3.505	-2.134	1.00	0.00

Figura: PDB não-alinhado

Arquivo PDB:

- Novo:

```
ATOM      1  N   TYR     1       0.115  -0.105   0.000  1.00  0.00
ATOM      2  CA  TYR     1       1.574  -0.047   0.000  1.00  0.00
ATOM      3  C   TYR     1       2.059   1.383   0.000  1.00  0.00
ATOM      4  O   TYR     1       1.281   2.336  -0.061  1.00  0.00
ATOM      5  CB  TYR     1       2.157  -0.753  -1.259  1.00  0.00
ATOM      6  CG  TYR     1       1.856  -2.248  -1.412  1.00  0.00
ATOM      7  CD1 TYR     1       2.567  -3.198  -0.673  1.00  0.00
ATOM      8  CD2 TYR     1       0.854  -2.668  -2.292  1.00  0.00
ATOM      9  CE1 TYR     1       2.273  -4.553  -0.810  1.00  0.00
ATOM     10  CE2 TYR     1       0.562  -4.022  -2.428  1.00  0.00
ATOM     11  CZ  TYR     1       1.272  -4.963  -1.686  1.00  0.00
ATOM     12  OH  TYR     1       0.985  -6.293  -1.815  1.00  0.00
ATOM     13 1H   TYR     1      -0.493   0.788   0.000  1.00  0.00
ATOM     14 2H   TYR     1      -0.421  -1.042   0.000  1.00  0.00
ATOM     15  HA  TYR     1       1.952  -0.534   0.918  1.00  0.00
ATOM     16 1HB  TYR     1       1.824  -0.213  -2.170  1.00  0.00
ATOM     17 2HB  TYR     1       3.258  -0.632  -1.277  1.00  0.00
ATOM     18  HD1 TYR     1       3.342  -2.888   0.014  1.00  0.00
ATOM     19  HD2 TYR     1       0.290  -1.942  -2.863  1.00  0.00
```

Figura: PDB alinhado

Arquivo PDB:

- Novo:

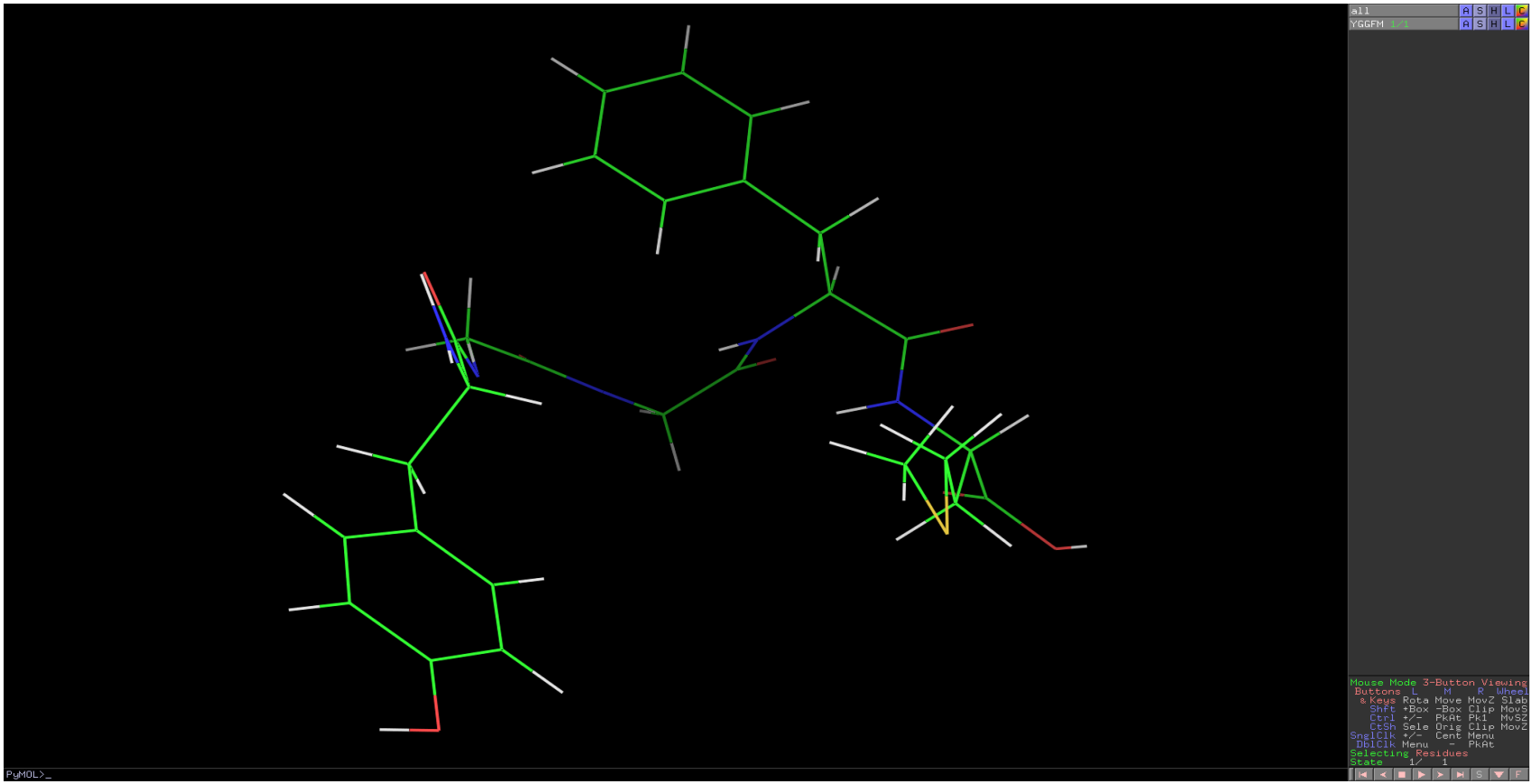


Figura: Estrutura PDB alinhado

NLYIQWLKDGGPSSGRPPPS

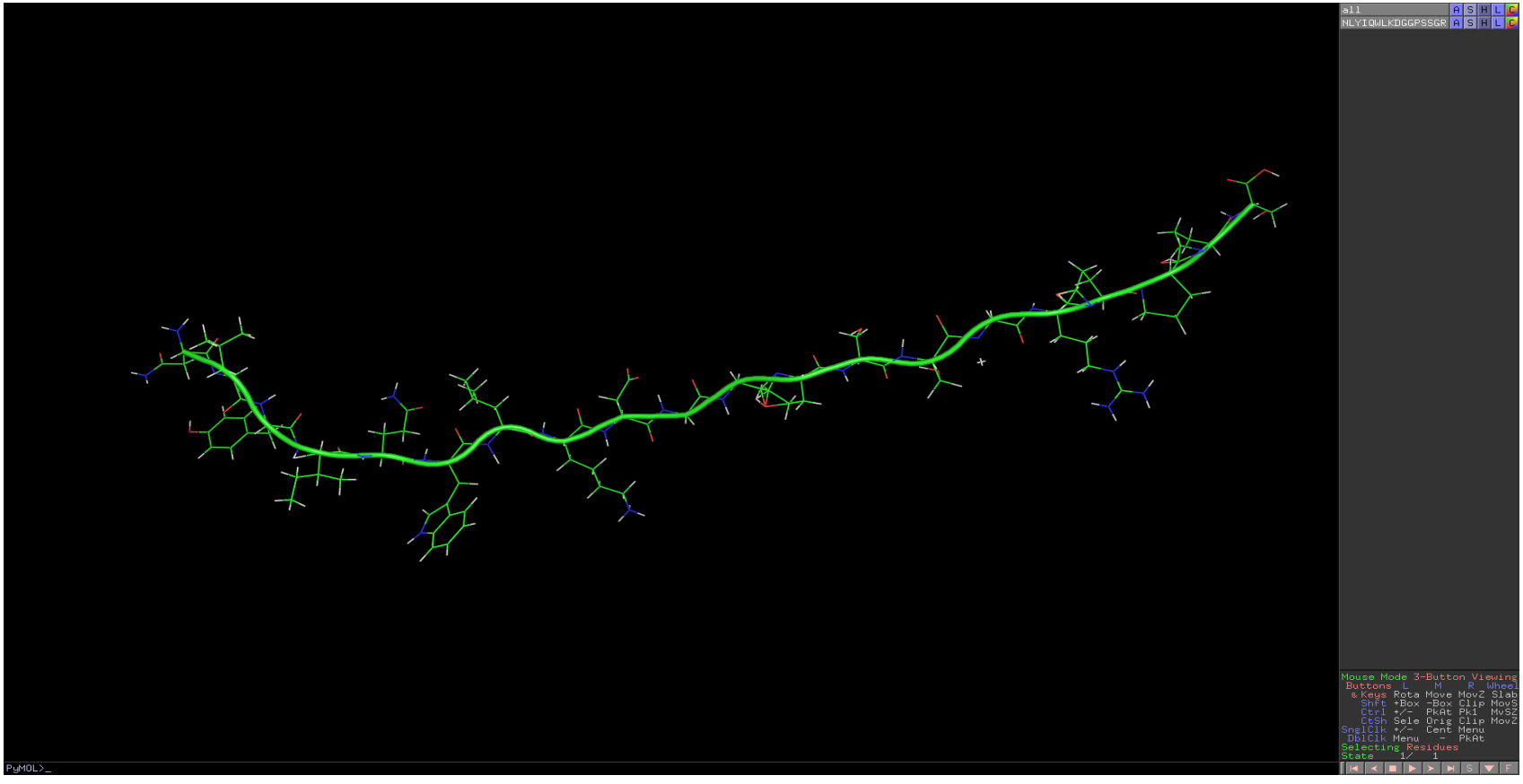


Figura: Estrutura PDB alinhado

Amino	Phi	Psi
ASN	360.00	180.00
LEU	-172.56	118.85
TYR	-138.80	-179.99
ILE	-92.39	179.98
GLN	179.67	180.00
TRP	-122.53	-179.98
LEU	-169.21	118.89
LYS	-115.19	-179.99
ASP	-173.21	-178.84
GLY	-163.79	180.00
GLY	178.21	-180.00
PRO	135.76	-179.96
SER	-178.65	180.00
SER	-139.24	-179.97
GLY	-170.36	179.99
ARG	125.59	178.80
PRO	150.60	-179.99
PRO	-169.66	179.97
PRO	146.27	-179.97
SER	-113.62	360.00

Figura: Angulos PHI e PSI iniciais

1L2Y-P

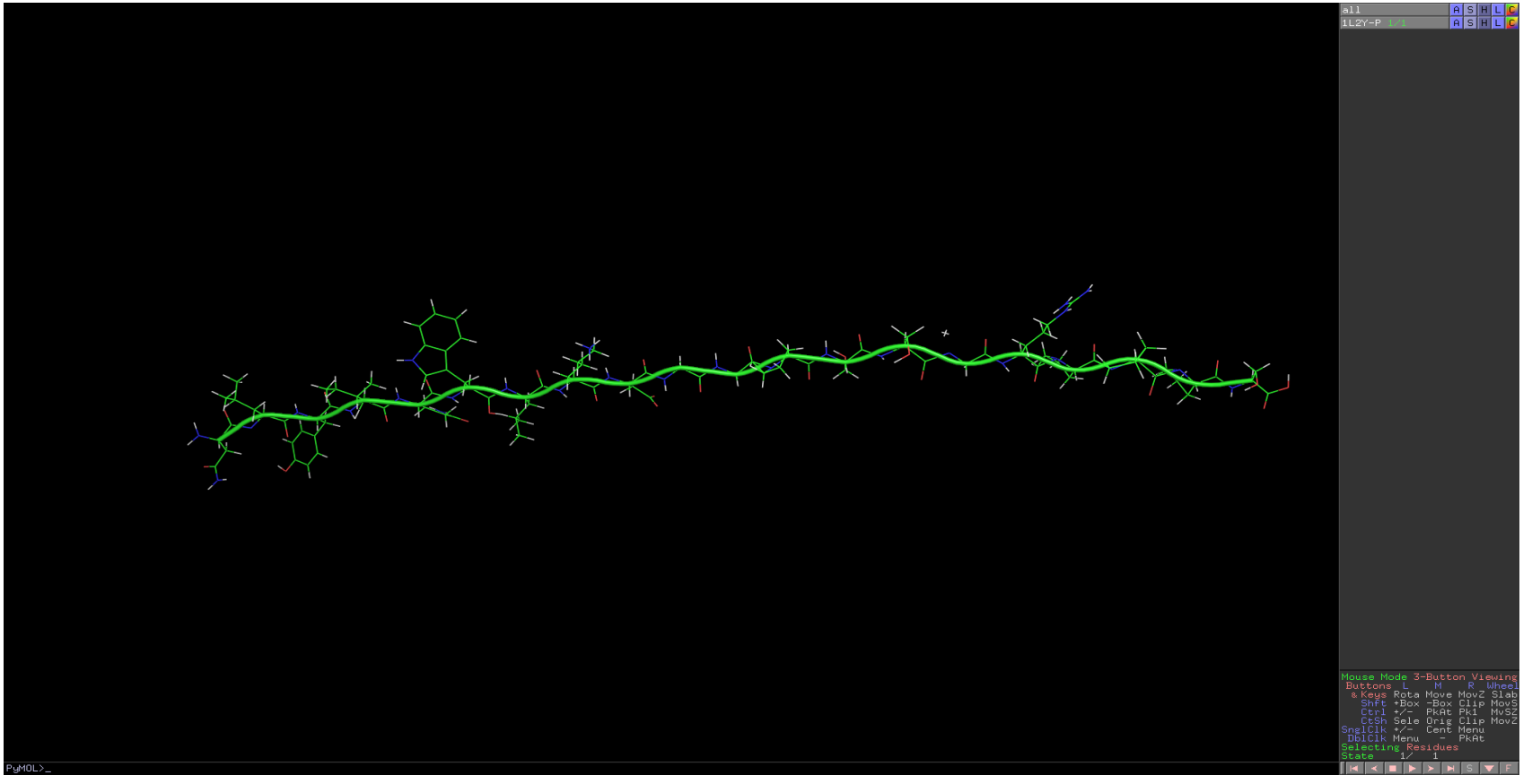


Figura: PHI e PSI em 180.

1L2Y-P x 1L2Y = 15.92

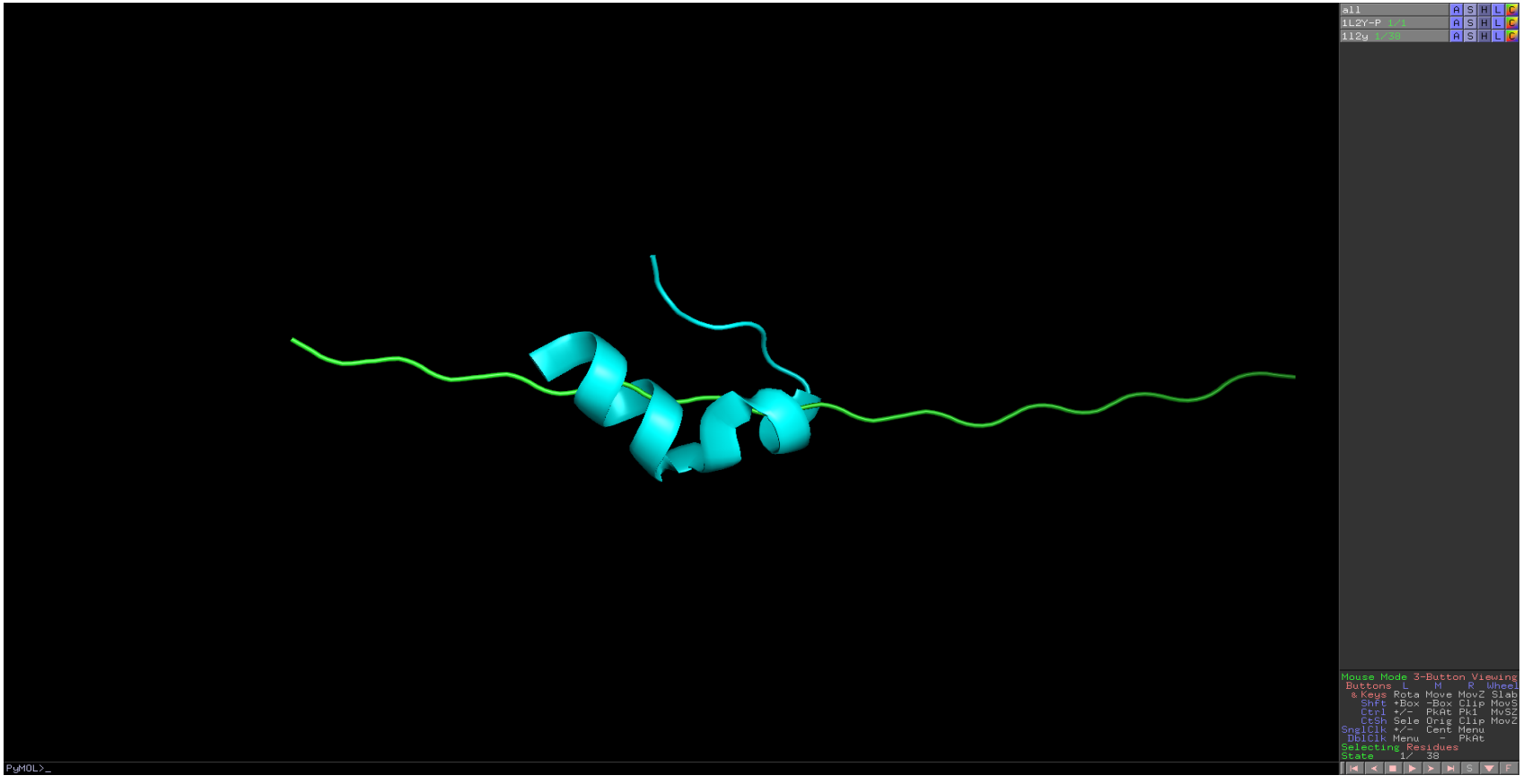


Figura: Alinhamento de estruturas

Amino	Phi	Psi
ASN	360.00	180.00
LEU	180.00	-180.00
TYR	179.98	-179.98
ILE	179.98	-179.99
GLN	179.97	179.94
TRP	-179.95	-179.98
LEU	180.00	-179.98
LYS	180.00	179.98
ASP	-179.96	179.99
GLY	179.98	-179.99
GLY	-179.99	-179.99
PRO	-179.96	-179.95
SER	179.97	179.99
SER	-179.99	-179.99
GLY	-179.99	-179.98
ARG	179.96	-180.00
PRO	-180.00	179.97
PRO	-179.97	-179.97
PRO	179.99	179.99
SER	179.99	360.00

Figura: Angulos PHI e PSI fixados em 180.

1L2Y-F x 1L2Y = 5.65

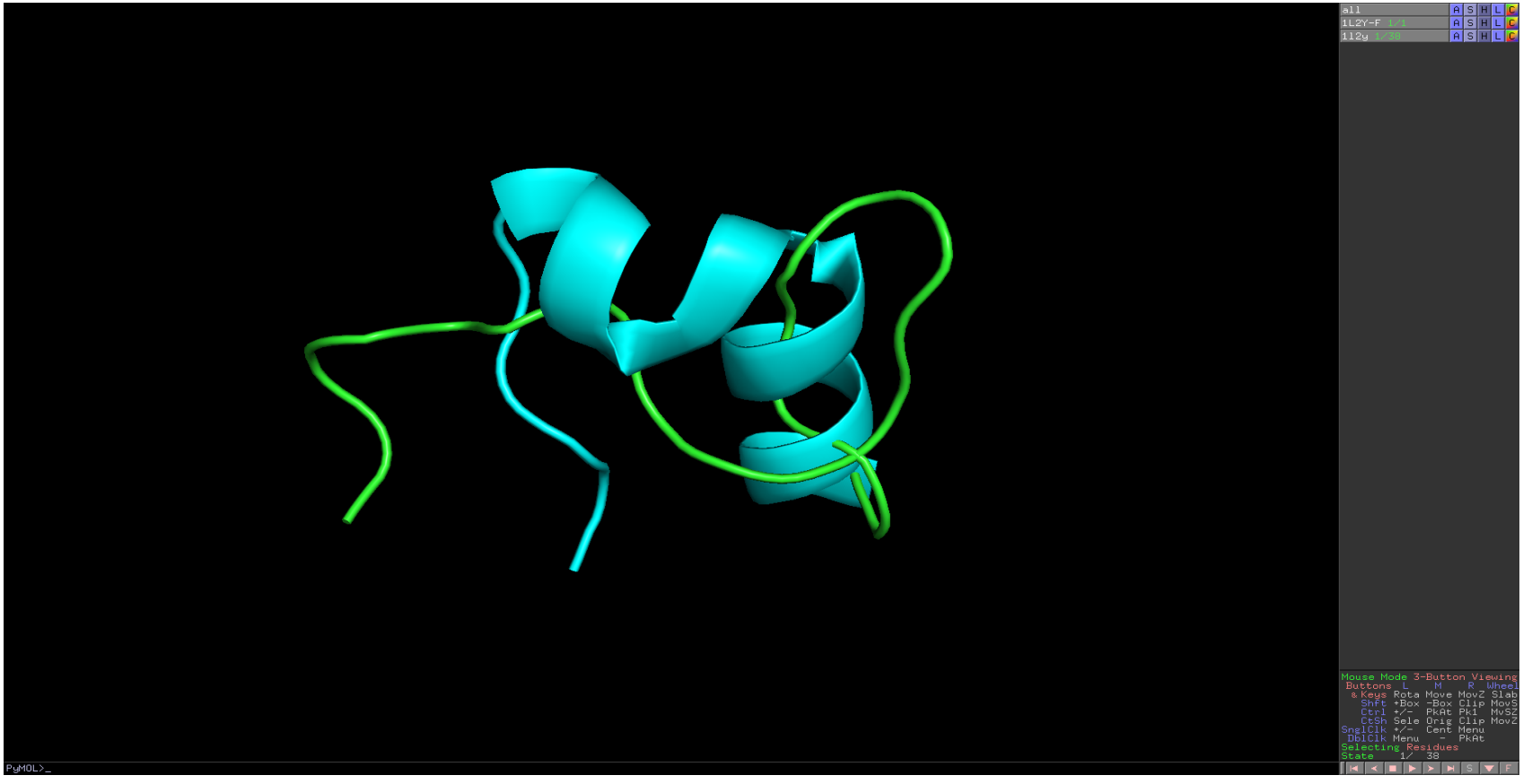


Figura: Alinhamento de estruturas

1L2Y-F x 1L2Y = 5.65

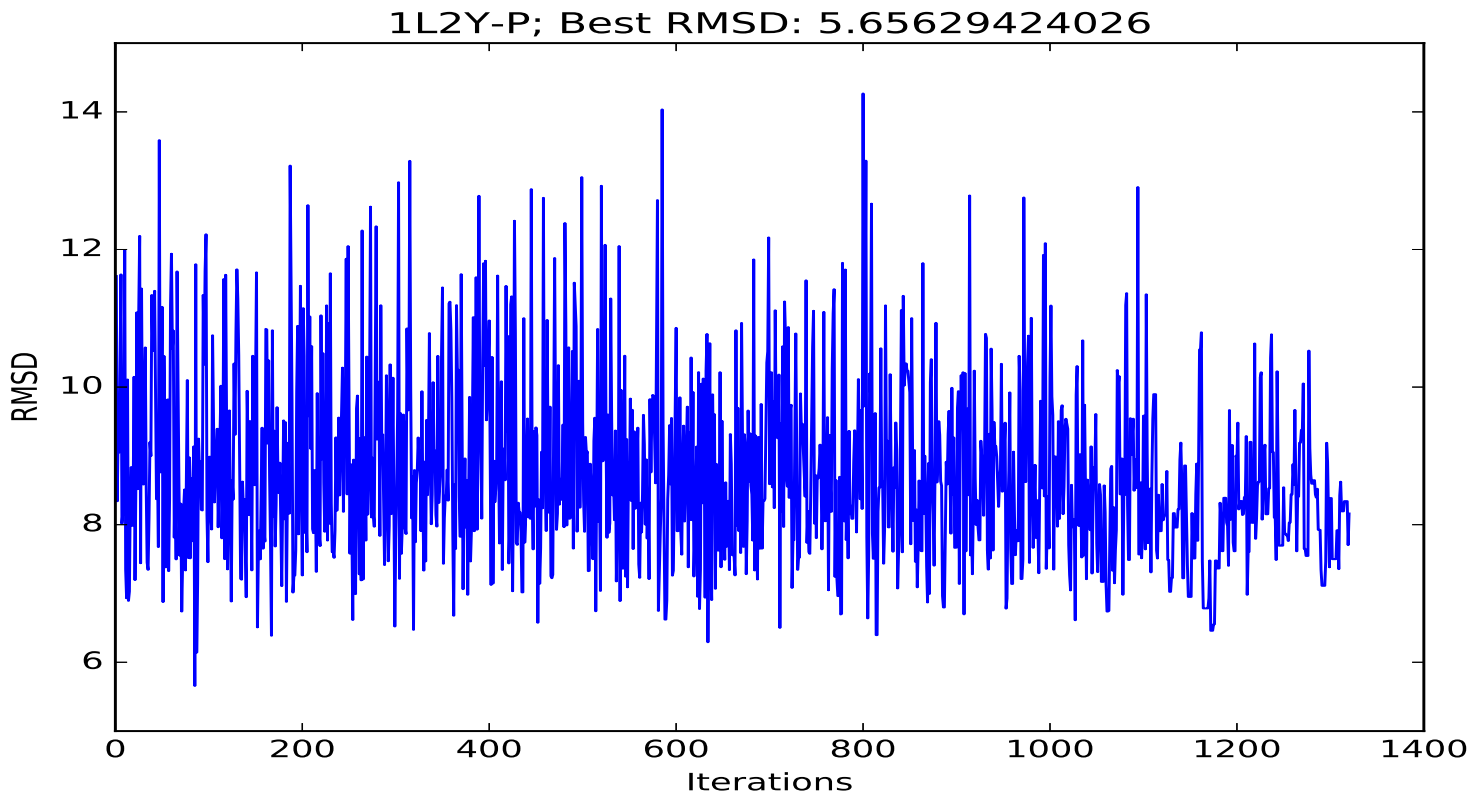


Figura: Alinhamento de estruturas