Evaluation in silico of the (pBthTX-I)$_2$K Peptide as a SARS-CoV-2 PL^{pro} Protease inhibitor

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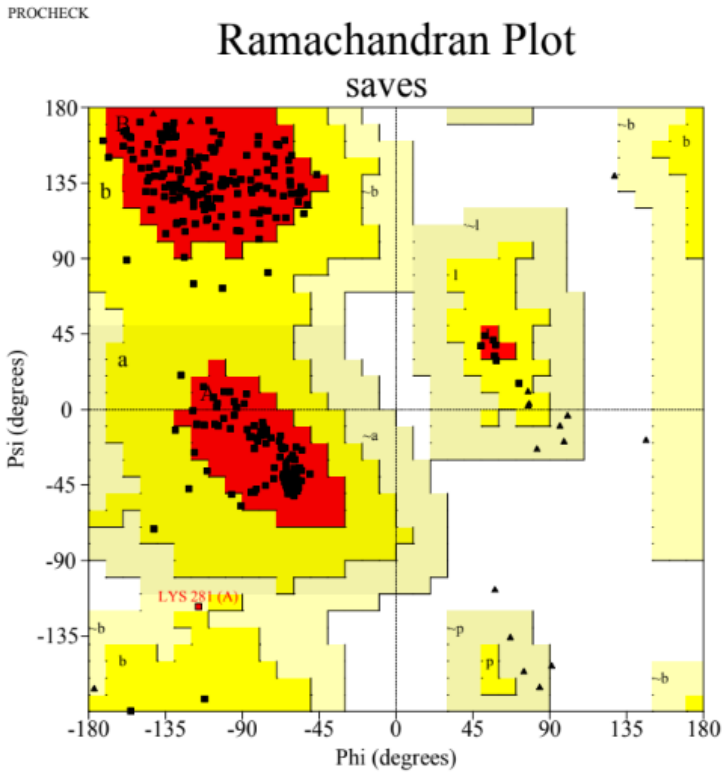

Fig. S1 Ramachandran Plot Analysis of the Protein Structure. This plot illustrates the conformational quality of the protein. The analysis shows that 93.6% of residues are in the core region, indicating favorable conformations, while 6.0% are allowed, 0.4% are general, and 0.0% are disallowed. A total of 7 residues (out of 314) are labeled for deviation from ideal positions, and 1 residue (out of 184) exhibits unusual chi1-chi2 angles. Side chain parameters reveal 5 better residues with no residues in worse conformations. Residue properties indicate a maximum deviation of 4.3 and no bad contacts, suggesting structural integrity. G-factor analysis shows dihedrals at -0.10, covalent at 0.07, and an overall score of -0.02. 88.7% of planar groups are within limits, while 11.3% require further investigation, and 4 residues fall off the graph. Overall, while the protein structure demonstrates good quality, specific residues and planar groups merit further examination.

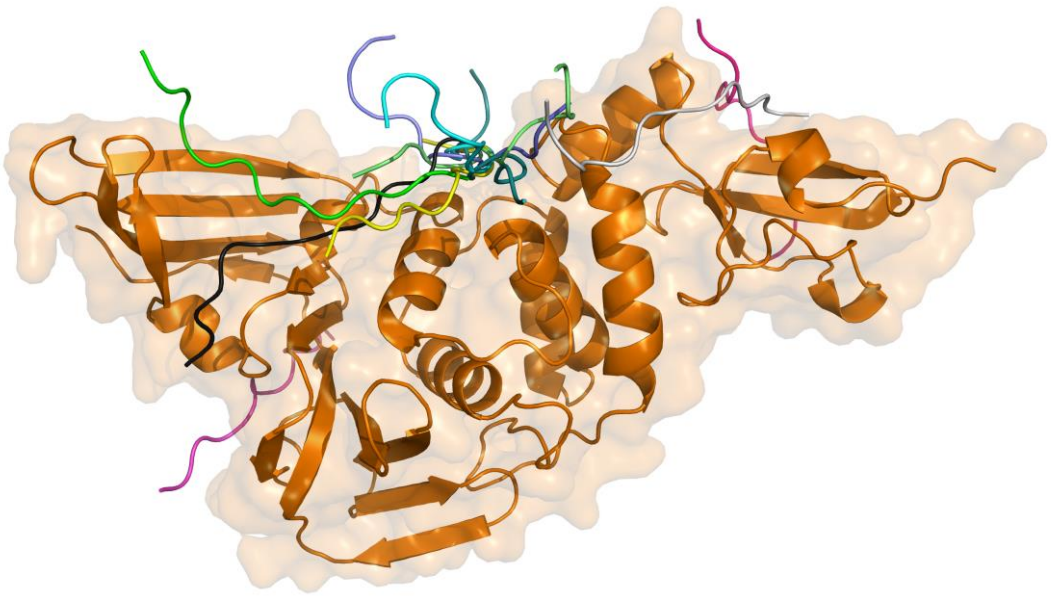

Figure S2: Representation of the orange MPL in surface format, highlighting the 10 best poses of the **BTX-MPL** complex: Pose 1 – light green; Pose 2 – cyan blue; Pose 3 – pink; Pose 4 – yellow; Pose 5 – gray; Pose 6 – purple; Pose 7 – black; Pose 8 – dark green; Pose 9 – dark blue; Pose 10 – dark pink.

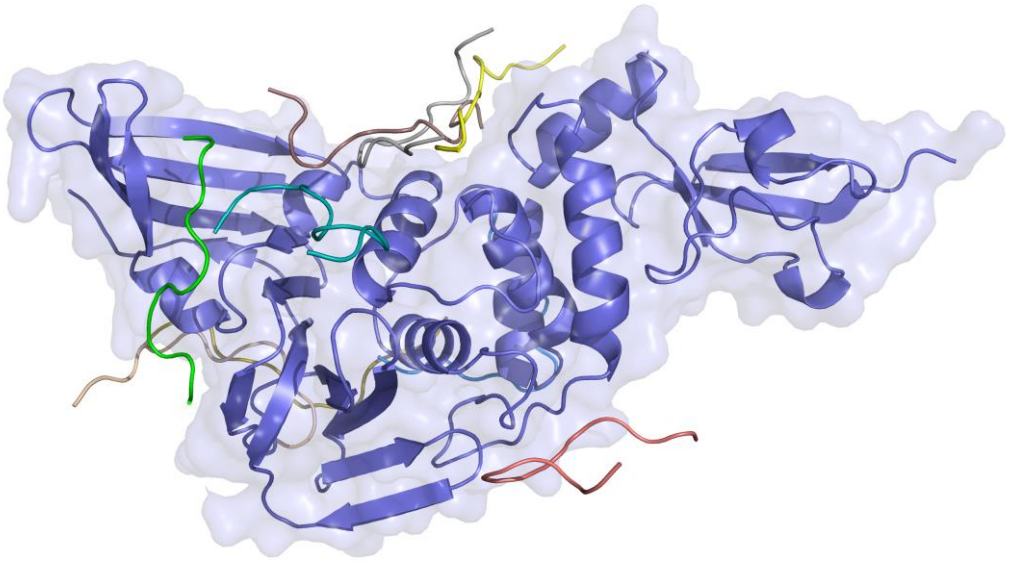

Figure S3: Representation of the blue CPL in surface format, highlighting the 10 best poses of the **BTX-CPL** complex: Pose 1 – light green; Pose 2 – gray; Pose 3 – light blue; Pose 4 – orange; Pose 5 – black; Pose 6 – cyan blue; Pose 7 – brown; Pose 8 – dark green; Pose 9 – dark pink; Pose 10 – dark yellow.

Table S1: HPEPDOCK Scoring Results for Molecular Docking Calculations for **BTX-MPL** (Includes 100 Poses Generated by HPEPDOCK)

Pose	**Score (kcal.mol^{-1})**	**Pose**	**Score (kcal.mol^{-1})**
1	-197.655	51	-161.274
2	-195.398	52	-161.270
3	-194.983	53	-161.043
4	-190.214	54	-161.026
5	-183.951	55	-160.799
6	-178.225	56	-160.727
7	-176.543	57	-160.528
8	-176.445	58	-160.434
9	-174.990	59	-160.418
10	-174.938	60	-159.979
11	-174.358	61	-159.903
12	-174.095	62	-159.823
13	-173.207	63	-159.286
14	-173.074	64	-159.244
15	-172.978	65	-159.150
16	-172.723	66	-158.727
17	-171.730	67	-158.662
18	-171.667	68	-158.518
19	-170.302	69	-158.511
20	-170.189	70	-158.427
21	-169.297	71	-158.196
22	-169.024	72	-157.964
23	-168.498	73	-157.749
24	-168.489	74	-157.500
25	-168.435	75	-157.478
26	-168.340	76	-157.194
27	-168.288	77	-157.144
28	-167.218	78	-156.850
29	-166.971	79	-156.639
30	-166.274	80	-156.627
31	-166.151	81	-156.493
32	-165.791	82	-156.413
33	-165.769	83	-156.209
34	-164.927	84	-156.169
35	-164.845	85	-156.165
36	-164.755	86	-155.979
37	-164.349	87	-155.967
38	-163.803	88	-155.704
39	-163.490	89	-155.654
40	-163.316	90	-155.597
41	-163.229	91	-155.430
42	-162.835	92	-155.433
43	-162.269	93	-155.376
44	-162.224	94	-155.257
45	-162.186	95	-155.222

Pose	Score (kcal.mol^{-1})	Pose	Score (kcal.mol^{-1})
46	-161.958	96	-155.100
47	-161.930	97	-154.906
48	-161.848	98	-154.831
49	-161.799	99	-154.822
50	-161.760	100	-154.821

Table S2: HPEPDOCK Scoring Results for Molecular Docking Calculations for **BTX-CPL** (Includes 100 Poses Generated by HPEPDOCK)

Pose	Score (kcal.mol^{-1})	Pose	Score (kcal.mol^{-1})
1	-197.014	51	-163.166
2	-190.734	52	-163.027
3	-188.331	53	-162.980
4	-187.479	54	-162.881
5	-186.657	55	-162.384
6	-185.605	56	-162.326
7	-183.848	57	-162.295
8	-182.384	58	-162.247
9	-182.144	59	-161.488
10	-181.576	60	-161.426
11	-180.441	61	-161.360
12	-178.435	62	-161.183
13	-178.354	63	-161.180
14	-177.357	64	-161.115
15	-174.201	65	-161.074
16	-174.079	66	-161.034
17	-173.216	67	-160.967
18	-172.480	68	-160.942
19	-172.331	69	-160.688
20	-170.775	70	-160.661
21	-170.604	71	-160.602
22	-170.492	72	-160.495
23	-170.430	73	-160.266
24	-169.733	74	-160.225
25	-169.270	75	-160.185
26	-169.090	76	-160.019
27	-169.016	77	-160.013
28	-168.739	78	-159.914
29	-167.682	79	-159.911
30	-167.575	80	-159.802
31	-166.968	81	-159.791
32	-166.900	82	-159.751
33	-166.864	83	-159.646
34	-166.853	84	-159.358
35	-166.784	85	-159.261

Pose	Score (kcal.mol^{-1})	Pose	Score (kcal.mol^{-1})
36	-166.366	86	-159.197
37	-166.250	87	-159.153
38	-166.051	88	-159.081
39	-165.792	89	-159.051
40	-165.788	90	-159.005
41	-165.732	91	-158.896
42	-165.107	92	-158.877
43	-164.856	93	-158.687
44	-164.799	94	-158.502
45	-164.802	95	-158.381
46	-164.404	96	-158.233
47	-164.319	97	-158.215
48	-163.836	98	-158.109
49	-163.593	99	-157.934
50	-163.379	100	-157.883