

Supporting Information for PETIMOT: A Novel Framework for Inferring Protein Motions from Sparse Data Using SE(3)-Equivariant Graph Neural Networks

A Statistical significance of method performance comparisons

Metrics	AlphaFlow	ESMFlow	NMA
Min. LS Error	2.24e-22	1.02e-33	6.45e-43
Min. Magnitude Error	4.83e-13	1.55e-24	7.44e-37
OLA LS Error	9.15e-26	6.59e-40	7.62e-44
OLA Magnitude Error	1.93e-11	2.22e-36	4.96e-47
Global SS Error	1.86e-28	1.49e-55	2.47e-50

Table SI.A.1: **Significance of the comparison between *PETIMOT-default* and baseline methods on the test set (824 proteins).** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. Significant p-values (<0.05) are highlighted in bold. The average performance values are reported in the main Table 1.

Metrics	5 layers	10 layers	shared 15 layers	reduced dim.
Min. LS Error	8.48e-06	0.72	0.84	0.53
Min. Magnitude Error	8.82e-11	0.15	5.04e-02	0.70
OLA LS Error	5.55e-11	0.63	0.28	0.67
OLA Magnitude Error	1.65e-10	0.12	2.08e-07	3.82e-02
Global SS Error	2.11e-36	1.36e-02	2.42e-05	5.86e-04

Table SI.A.2: **Significance of the network depth ablations performed on *PETIMOT-default* assessed on the test set (824 proteins).** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. The cumulative performance curves are shown in Figure B.1.

Metrics	ESMC (600M)	sequence ablation (w. rand emb.)	structure ablation (ProstT5)	seq. & struct. ablation	
Min. LS Error	2.57e-02	1.12e-09	3.47e-25	3.88e-80	2.70e-107
Min. Magnitude Error	0.26	1.41e-05	1.20e-32	2.49e-100	2.00e-107
OLA LS Error	0.13	2.09e-08	1.25e-32	2.18e-95	2.24e-116
OLA Magnitude Error	0.11	1.91e-04	4.10e-32	1.00e-120	1.39e-116
Global SS Error	1.77e-03	8.55e-14	9.55e-70	1.12e-105	2.75e-122

Table SI.A.3: **Significance of the structure and sequence information ablations performed on *PETIMOT-default* assessed on the test set (824 proteins).** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. The cumulative performance curves are shown in Figure B.2.

Metrics	only random	only close	fixed random
Min. LS Error	5.09e-04	1.84e-04	0.88
Min. Magnitude Error	3.05e-03	1.23e-03	0.66
OLA LS Error	2.26e-04	1.55e-16	0.91
OLA Magnitude Error	4.61e-04	6.94e-09	1.69e-02
Global SS Error	1.07e-08	2.42e-45	2.15e-02

Table SI.A.4: **Significance of the graph connectivity ablations performed on *PETIMOT-default* assessed on the test set (824 proteins).** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. Significant p-values (<0.05) are highlighted in bold. The cumulative performance curves are shown in Figure B.4.

Metrics	AlphaFlow	ESMFlow	NMA
Min. LS Error	2.98e-13	9.07e-24	3.36e-30
Min. Magnitude Error	1.64e-06	2.25e-16	5.68e-24
OLA LS Error	1.49e-15	1.68e-29	8.11e-29
OLA Magnitude Error	3.89e-07	6.23e-29	2.46e-36
Global SS Error	1.82e-16	1.35e-40	1.98e-34

Table SI.A.5: **Significance of the comparison between *PETIMOT-stringent* and baseline methods on the non-redundant test set (734 proteins).** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. Significant p-values (<0.05) are highlighted in bold. The cumulative performance curves are shown in Figure C.4a-b.

Metrics	<i>PETIMOT-default</i>	AlphaFlow	ESMFlow	NMA
Min. LS Error	0.62	1.26e-08	7.98e-15	2.24e-17
Min. Magnitude Error	1.00	1.90e-03	2.71e-08	2.22e-12
OLA LS Error	0.75	9.02e-10	4.00e-16	4.26e-16
OLA Magnitude Error	0.98	1.48e-03	1.00e-16	3.13e-21
Global SS Error	0.99	1.54e-09	4.75e-23	1.69e-18

Table SI.A.6: **Significance of the comparison between *PETIMOT-stringent* and baseline methods on 474 test proteins that share less than 30% sequence similarity with any protein used in training or validation of either model.** We report the p-value of the one-sided paired Wilcoxon ranked signed test for each pair of methods (X,Y) where X is *PETIMOT-default* and the alternative hypothesis is that performance of X is better than than of Y, for different performance metrics. Significant p-values (<0.05) are highlighted in bold. The cumulative performance curves are shown in Figure C.4c-d.

B Influence of initial random seeding for predicting motions

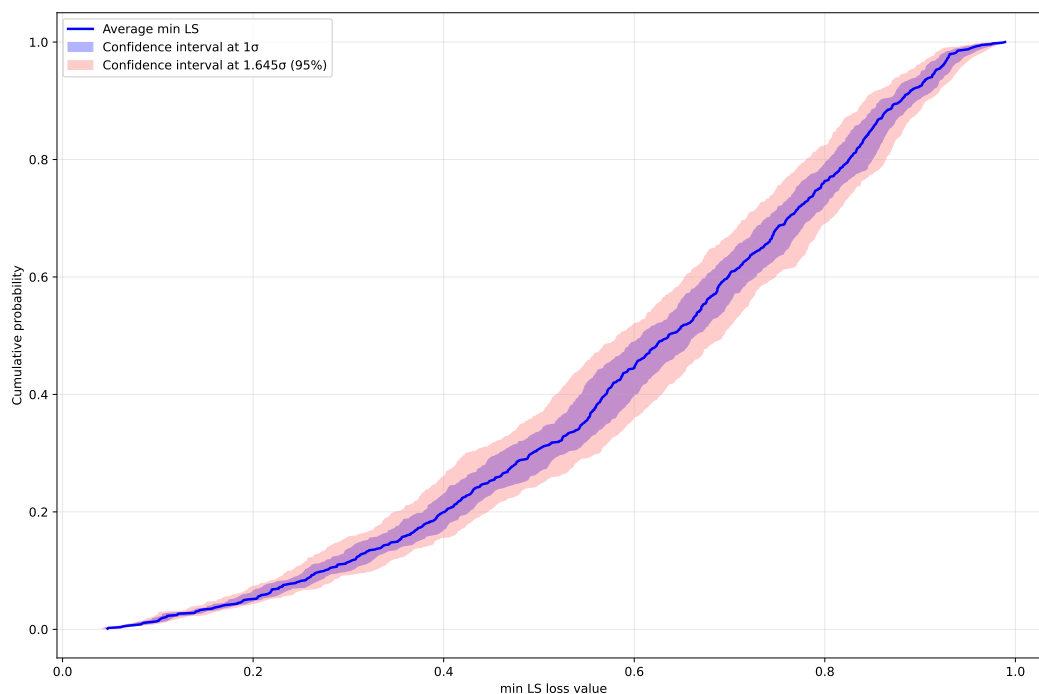


Figure SI.B.1: **Cumulative distribution analysis of PETIMOT robustness across random seeds on the test set (824 proteins).** The blue curve shows the cumulative distribution of minimum LS errors averaged over 100 training runs with different seeds (ranging from 1 to 100). The x-axis represents the loss values, and the y-axis indicates the cumulative probability. The blue and red confidence intervals correspond to 1σ and 1.645σ (95% quantile), respectively. This cumulative analysis provides a comprehensive view of the error distribution and confirms the robustness of our protein motion inference approach across different random initializations.

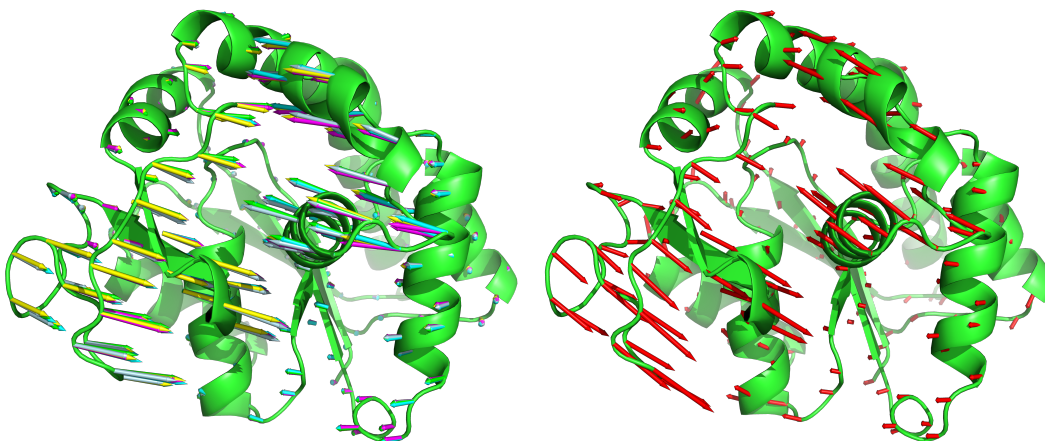


Figure SI.B.2: Correct predictions of motions along the first principal component for chain A of PDB ID 1AKE. The mean min LS loss is 0.29. Predictions for five random seeds are shown in the left (with different colors). Ground-truth motions are shown in the right. One can see consistent predictions over arbitrary seeds.

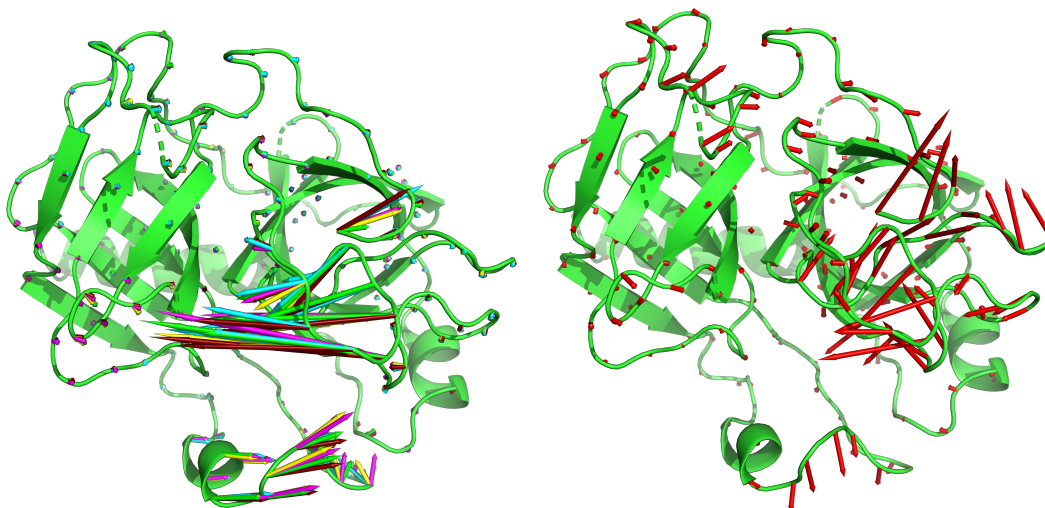


Figure SI.B.3: Incorrect predictions of motions along the first principal component for chain P of PDB ID 2ZCH. The mean min LS loss is 0.83. Predictions for five random seeds are shown in the left (with different colors). Ground-truth motions are shown in the right. One can see consistent, even though incorrect, predictions over arbitrary seeds.