

Supporting Information

*PCAViz: An Open-Source Python/JavaScript Toolkit
for Visualizing Molecular Dynamics Simulations in
the Web Browser*

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Table S1. PCAViz accuracy when applied to a LARP1 simulation. Using various cumulative-variance and rounding-precision parameters, we compressed a 100-frame simulation of LARP1 (1,326 non-hydrogen atoms) with the PCAViz Compressor. We then decompressed each simulation to recover the atomic Cartesian coordinates. To judge PCAViz accuracy, we calculated the average RMSD (plus or minus the standard deviation) between each frame of the original trajectory and the corresponding frame of the PCAViz-processed trajectory. We also include the file size of each output JSON file so users can judge the extent of compression. The number of top components that PCAViz retained in order to account for the user-specified cumulative-variance cutoff is given in parentheses.

Cumulative-Variance Cutoff (Number of Components)	Precision: Tenth	Precision: Hundredth	Precision: Thousandth
20% (1)	1.55 Å ± 0.18 48K	1.47 Å ± 0.18 56K	1.46 Å ± 0.18 65K
25% (1)	1.55 Å ± 0.18 48K	1.47 Å ± 0.18 56K	1.46 Å ± 0.18 65K
30% (2)	1.54 Å ± 0.17 56K	1.38 Å ± 0.14 66K	1.37 Å ± 0.14 78K
40% (3)	1.52 Å ± 0.17 64K	1.32 Å ± 0.12 75K	1.30 Å ± 0.12 89K
50% (5)	1.49 Å ± 0.16 81K	1.23 Å ± 0.10 94K	1.20 Å ± 0.10 111K
60% (9)	1.45 Å ± 0.16 113K	1.10 Å ± 0.080 131K	1.08 Å ± 0.080 157K
70% (15)	1.42 Å ± 0.16 162K	0.99 Å ± 0.054 188K	0.95 Å ± 0.056 227K
75% (20)	1.41 Å ± 0.16 203K	0.91 Å ± 0.049 235K	0.87 Å ± 0.052 285K
80% (27)	1.39 Å ± 0.16 260K	0.82 Å ± 0.040 300K	0.77 Å ± 0.044 365K
90% (48)	1.36 Å ± 0.16 431K	0.62 Å ± 0.038 497K	0.55 Å ± 0.046 608K
100% (99)	1.34 Å ± 0.16 845K	0.31 Å ± 0.033 978K	0.032 Å ± 0.0035 1.2 M

Table S2. PCAViz accuracy when applied to a TEM-1 simulation. Using various cumulative-variance and rounding-precision parameters, we compressed a 1,000-frame simulation of TEM-1 β -lactamase (2,030 non-hydrogen atoms) with the PCAViz Compressor. We then decompressed each simulation to recover the atomic Cartesian coordinates. To judge PCAViz accuracy, we calculated the average RMSD (plus or minus the standard deviation) between each frame of the original trajectory and the corresponding frame of the PCAViz-processed trajectory. We also include the file size of each output JSON file so users can judge the extent of compression. The number of top components that PCAViz retained in order to account for the user-specified cumulative-variance cutoff is given in parentheses.

Cumulative-Variance Cutoff (Number of Components)	Precision: Tenth	Precision: Hundredth	Precision: Thousandth
20% (2)	0.92 Å \pm 0.068 94K	0.85 Å \pm 0.056 111K	0.85 Å \pm 0.056 131K
25% (4)	0.92 Å \pm 0.068 125K	0.82 Å \pm 0.053 147K	0.81 Å \pm 0.053 174K
30% (5)	0.91 Å \pm 0.069 141K	0.80 Å \pm 0.052 165K	0.79 Å \pm 0.052 196K
40% (10)	0.90 Å \pm 0.070 217K	0.75 Å \pm 0.047 254K	0.74 Å \pm 0.048 303K
50% (19)	0.89 Å \pm 0.070 354K	0.69 Å \pm 0.037 412K	0.67 Å \pm 0.038 497K
60% (34)	0.88 Å \pm 0.071 581K	0.62 Å \pm 0.031 676K	0.60 Å \pm 0.031 818K
70% (61)	0.86 Å \pm 0.072 988K	0.55 Å \pm 0.023 1.2M	0.52 Å \pm 0.023 1.4M
75% (84)	0.86 Å \pm 0.072 1.4M	0.51 Å \pm 0.020 1.6M	0.48 Å \pm 0.019 1.9M
80% (115)	0.86 Å \pm 0.073 1.8M	0.47 Å \pm 0.017 2.1M	0.43 Å \pm 0.016 2.5M
90% (240)	0.85 Å \pm 0.073 3.6M	0.36 Å \pm 0.013 4.2M	0.30 Å \pm 0.0089 5.2M
100% (1000)	0.84 Å \pm 0.074 15M	0.21 Å \pm 0.016 17M	0.021 Å \pm 0.0017 21M