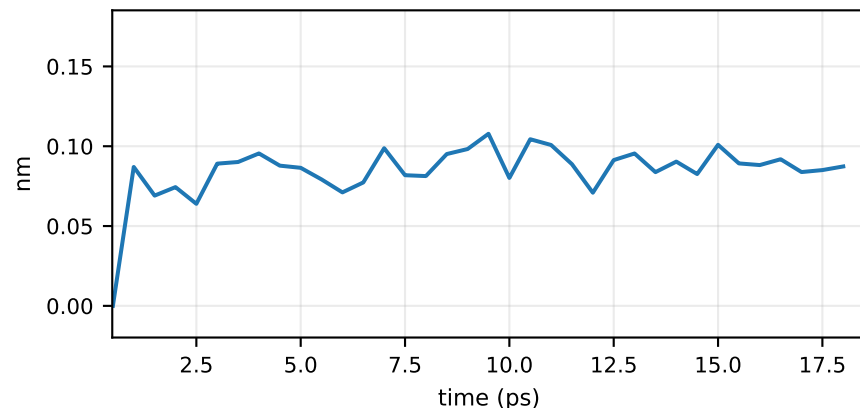
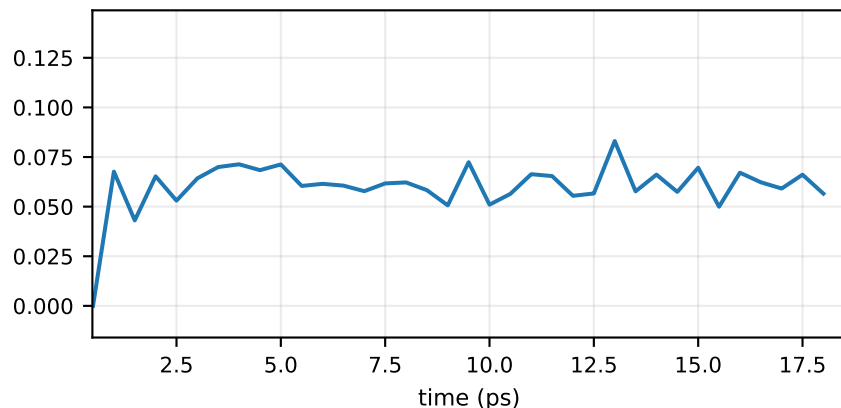


D Ligand 03P in the pocket. Top row NEW (0.5-18 ps), bottom row UPSTREAM (10-1000 ps): separate time axes, each column shares its Y scale between the rows. No binding threshold line is drawn in these panels. Each trajectory is referenced to its OWN first analysed frame; the two must not be subtracted. Frame 1 is the reference, so its value is 0 by definition.

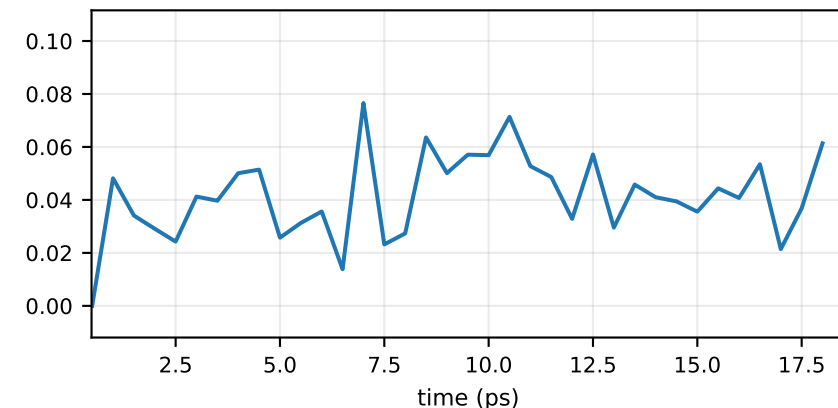
D1 Ligand RMSD in the RECEPTOR frame
(displacement, receptor-fitted)
NEW · 0.5-18 ps (36 frames)



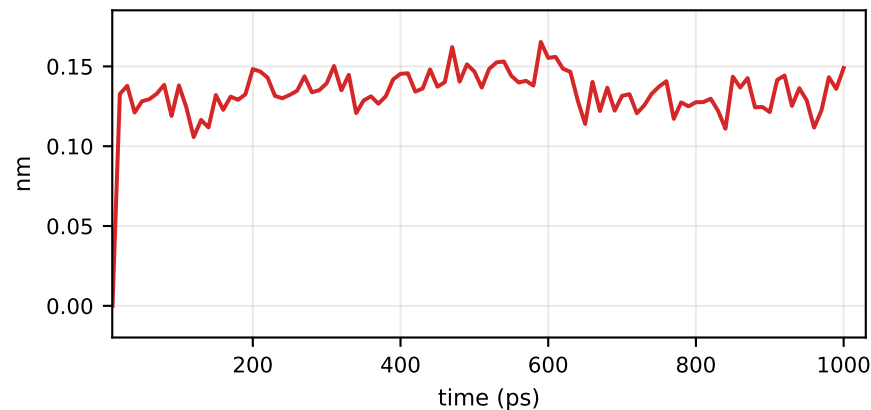
D2 Ligand INTERNAL RMSD
(shape only, ligand-fitted)
NEW · 0.5-18 ps (36 frames)



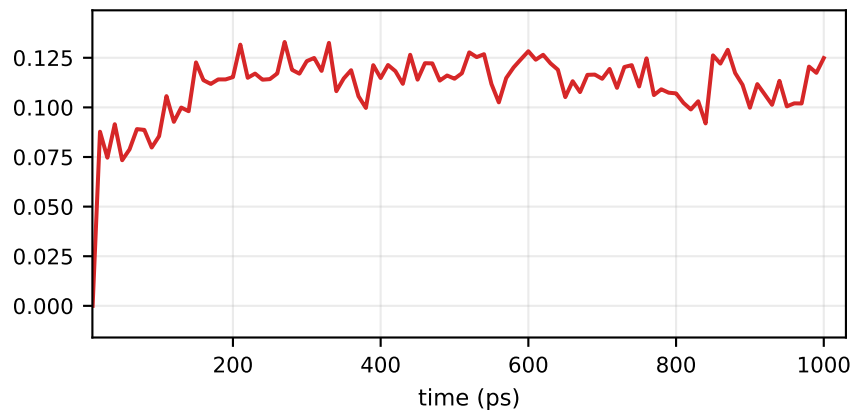
D3 Net centroid displacement
NEW · 0.5-18 ps (36 frames)



UPSTREAM · 10-1000 ps (100 frames)



UPSTREAM · 10-1000 ps (100 frames)



UPSTREAM · 10-1000 ps (100 frames)

