

[illegible]

	10.5281/zenodo.7125978 - Single molecule FRET data, Zenodo: 10.5281/zenodo.7125978 - Single molecule FRET data, Zenodo: 10.5281/zenodo.7125978 - Single molecule FRET data, Zenodo: 10.5281/zenodo.7125978 - Integrative model, Zenodo: 10.5281/zenodo.7125978 - Comparative model, Zenodo: 10.5281/zenodo.7125978 - Experimental model, Zenodo: 10.5281/zenodo.7125978 - Experimental model, Zenodo: 10.5281/zenodo.7125978
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	2
Number of models in ensembles	4325, 114
Number of deposited models	200
Model precision (uncertainty of models)	- Not available - Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 4.23-11.19 - Ramachandran outliers: 11-23 - Sidechain outliers: 49-80
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	

1. Name	Unbiased DMD Simulations
Method	DMD simulations
Number of computed models	20871
2. Name	FRET-guided screening of structures from molecular dynamics simulations
Method	None
Number of computed models	4439
Software	- AvTraj (version 0.0.9) - pDMD (version 1.100)