

[*Datasets used for modeling*](#)

- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- Single molecule FRET data, File: 10.5281/zenodo.6640962
- De Novo model, File: 10.5281/zenodo.6640962
- De Novo model, File: 10.5281/zenodo.6640962
- De Novo model, File: 10.5281/zenodo.6640962
- De Novo model, File: 10.5281/zenodo.6640962

2. Representation	
<i>Resolution</i>	Atomic
<i>Number of rigid bodies, flexible units</i>	8, 0

<i>Rigid bodies</i>	- A: 1-16, 17-37 - B: 1-21, 22-37 - C: 1-16, 17-32 - D: 1-16, 17-32
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	
4. Validation	
<i>Number of ensembles</i>	2
<i>Number of models in ensembles</i>	7, 3
<i>Number of deposited models</i>	10
<i>Model precision (uncertainty of models)</i>	None, Å, None, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	- Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-2: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-3: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-4: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-5: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-6: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-7: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-8: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-9: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-10: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0
<i>Model quality: assessment of excluded volume</i>	Not applicable

<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Method</i>	Rigid body docking
<i>Name</i>	None
<i>Number of computed models</i>	1000
2. <i>Method</i>	Refinement
<i>Name</i>	None
<i>Number of computed models</i>	1000
3. <i>Method</i>	Error estimation (Bootstrapping)
<i>Name</i>	None
<i>Number of computed models</i>	100
4. <i>Method</i>	Rigid body docking
<i>Name</i>	None
<i>Number of computed models</i>	1000
5. <i>Method</i>	Refinement
<i>Name</i>	None
<i>Number of computed models</i>	1000
6. <i>Method</i>	Error estimation (Bootstrapping)
<i>Name</i>	None
<i>Number of computed models</i>	100
7. <i>Method</i>	Refinement by restrained MD
<i>Name</i>	MD simulations
<i>Number of computed models</i>	10000

Software

- [FPS \(FRET Positioning and Screening\)](#) (version 1.100)
- [Paris](#) (version Not available)
- [Tatiana](#) (version Not available)
- Python_clustering_script (version Not available)
- [Amber_11](#) (version Not available)