

	<ul style="list-style-type: none"> - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Single molecule FRET data, File: 10.5281/zenodo.7125978 - Other, File: 10.5281/zenodo.7125978 - Other, File: 10.5281/zenodo.7125978 - Other, File: 10.5281/zenodo.7125978 - Other, File: 10.5281/zenodo.7125978 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 1KJW - Experimental model, PDB ID: 6QJD - Integrative model, Not available - Other, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	1, 0
Rigid bodies	A: 313-724
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 4 unique PredictedContactRestraint: Lower Upper Bound Distance: 2.0-3.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	4
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed

Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Model-1: Clashscore = 7.25, Number of Ramachandran outliers = 12, Number of sidechain outliers = 57 - Model-2: Clashscore = 8.23, Number of Ramachandran outliers = 12, Number of sidechain outliers = 56 - Model-3: Clashscore = 7.08, Number of Ramachandran outliers = 12, Number of sidechain outliers = 57 - Model-4: Clashscore = 8.07, Number of Ramachandran outliers = 12, Number of sidechain outliers = 57
Model quality: assessment of excluded volume	Not applicable
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. Method	FRET-guided rigid body docking
Name	None
2. Method	FRET-guided rigid body docking with disulfide mapping restraints
Name	None
Software	FRET Positioning and Screening (FPS) (version 1.100)