Summary of integrative structure determination of Structures of multiple states of the hGBP1 resolved by FRET, SAXS, and EPR (PDB ID: 9A1G, PDB-Dev ID: PDBDEV_00000088)

1. Model Composition	
Entry composition	hGBP1 wildtype: chain(s) A (583 residues)

Datasets used for modeling	- Experimental model, PDB: 1DG3 - SAS data, SASBDB: SASDDD6 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - Ensemble FRET data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - EPR data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557 - Single molecule FRET data, Zenodo: 10.5281/zenodo.6534557
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	100, 106
Number of deposited models	206
Model precision (uncertainty of models)	- Not available - Not available
Data quality	SASDDD6: Rg from Gunier is 3.89nm and Rg from p(r) is 4.02nm
Model quality: assessment of atomic segments	- Clashscore: 0.21-5.21 - Ramachandran outliers: 2-19 - Sidechain outliers: 8-123
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	Rigid body docking
2. Name	Targeted NMSim
3. Name	MD simulation
Software	- FPS (version Not available) - NMSim (version Not available) - Amber 14 (version Not available) - DeerAnalysis2006 (version Not available)