

Summary of integrative structure determination of Molten Globule Ensemble from Helicobacter pylori Flavodoxin (PDB ID: 9A1S, PDB-Dev ID: PDBDEV_00000112)

1. Model Composition	
Entry composition	MOLTEN GLOBULE OF APOFLAVODOXIN FROM HELICOBACTER PYLORI, ELECTRON TRANSPORT: chain(s) A (163 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 2BMV - Mutagenesis data, Not available - Other, Not available - Other, Not available
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	1
Number of models in ensembles	10
Number of deposited models	10
Model precision (uncertainty of models)	7.04, Å
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 1.66-6.64 - Ramachandran outliers: 6-14 - Sidechain outliers: 3-10
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. <i>Name</i>	Generation of the initial ensemble
<i>Method</i>	Biased (experimental phi-values) molecular dynamics simulations
<i>Description</i>	Experimental phi-values from mutagenesis experiments are used as a reaction coordinate to bias a starting model using molecular dynamics simulations (HQBMM module from Charmm program)
<i>Number of computed models</i>	21
2. <i>Name</i>	Ensemble refinement
<i>Method</i>	Ensemble refinement based on experimental spectroscopic data
<i>Description</i>	A variety of spectroscopic data (fluorescence, far- and near-UV, and NMR) used for refining the initial biased MD ensemble
<i>Number of computed models</i>	10
<i>Software</i>	CHARMM (version v.44b2)