

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

1. Model Composition	
<i>Entry composition</i>	MOLTEN GLOBULE OF APOFLAVODOXIN FROM HELICOBACTER PYLORI, ELECTRON TRANSPORT: Chain A (163 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 2BMV - Mutagenesis data, Not available - Other, Not available - Other, Not available
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of rigid bodies, flexible units</i>	0, 1
<i>Flexible units</i>	A: 1-163
<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>	1
<i>Number of models in ensembles</i>	10
<i>Number of deposited models</i>	10
<i>Model precision (uncertainty of models)</i>	7.04, Å
<i>Data quality</i>	Data quality has not been assessed

	<ul style="list-style-type: none"> - Model-1: Clashscore = 4.15, Number of Ramachandran outliers = 12, Number of sidechain outliers = 9 - Model-2: Clashscore = 5.4, Number of Ramachandran outliers = 11, Number of sidechain outliers = 5 - Model-3: Clashscore = 3.32, Number of Ramachandran outliers = 6, Number of sidechain outliers = 8 - Model-4: Clashscore = 5.82, Number of Ramachandran outliers = 12, Number of sidechain outliers = 6 - Model-5: Clashscore = 1.66, Number of Ramachandran outliers = 7, Number of sidechain outliers = 8 - Model-6: Clashscore = 7.06, Number of Ramachandran outliers = 14, Number of sidechain outliers = 10 - Model-7: Clashscore = 3.32, Number of Ramachandran outliers = 8, Number of sidechain outliers = 8 - Model-8: Clashscore = 2.91, Number of Ramachandran outliers = 9, Number of sidechain outliers = 8 - Model-9: Clashscore = 6.23, Number of Ramachandran outliers = 6, Number of sidechain outliers = 7 - Model-10: Clashscore = 6.23, Number of Ramachandran outliers = 11, Number of sidechain outliers = 3
<i>Model quality: assessment of atomic segments</i>	
<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	
<i>1. Method</i>	Generation of the initial ensemble
<i>Name</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 (HQBM module from Charmm program)
<i>Number of computed models</i>	21
<i>2. Method</i>	Ensemble refinement
<i>Name</i>	Ensemble refinement based on experimental spectroscopic data

<u>Description</u>	A variety of spectroscopic data (fluorescence, far- and near-UV, and NMR) used for refining the initial biased MD ensemble
<u>Number of computed models</u>	10
<u>Software</u>	CHARMM (version v.44b2)