

## Summary of integrative structure determination of Complex structure of holo-GmHO-1 and Ferredoxin III from maize root (PDB ID: 9A8X)

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Heme oxygenase (biliverdin-producing): chain(s) A (211 residues)</li> <li>- Ferredoxin-3, chloroplastic: chain(s) B (97 residues)</li> <li>- FE2/S2 (INORGANIC) CLUSTER: chain(s) C</li> <li>- PROTOPORPHYRIN IX CONTAINING FE: chain(s) D</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- NMR data, BMRB: <a href="#">26301</a></li> <li>- Experimental model, PDB: <a href="#">7CKA</a></li> <li>- Experimental model, PDB: <a href="#">5H57</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	0, 2
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	3
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 11.00-15.68</li> <li>- Ramachandran outliers: 0-2</li> <li>- Sidechain outliers: 9-14</li> </ul>
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	

<i>1. Name</i>	docking
<i>Description</i>	A docking simulation was performed with holo-GmHO-1 (Protein Data Bank [PDB] ID:7CKA) and maize Fd (Protein Data Bank [PDB] ID: 5h57) using the HADDOCK server based on NMR chemical shift perturbation experiments of apo-GmHO-1. Ten HADDOCK models were successfully obtained, from which the top cluster of models with a HADDOCK score of -57.0 +/- 2.2 were adopted.
<i>Software</i>	<a href="#">HADDOCK</a> (version 2.4)