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

1. Model Composition	
Entry composition	- Heme oxygenase (biliverdin-producing): Chain A (211 residues) - FE2/S2 (INORGANIC) CLUSTER: Chain C (Not available residues) - Ferredoxin-3, chloroplastic: Chain B (97 residues) - PROTOPORPHYRIN IX CONTAINING FE: Chain D (Not available residues)
Datasets used for modeling	- NMR data, BMRB: 26301 - Experimental model, PDB ID: 7CKA - Experimental model, PDB ID: 5H57
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 4
Flexible units	- B: 1-97 - A: 1-211 - C: None-None - D: None-None
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	3
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	- Model-1: Clashscore = 12.43, Number of Ramachandran outliers = 2, Number of sidechain outliers = 14 - Model-2: Clashscore = 11.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 9 - Model-3: Clashscore = 15.69, Number of Ramachandran outliers = 0, Number of sidechain outliers = 10
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	docking
Name	None
Description	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.
Software	HADDOCK (version 2.4)