Summary of integrative structure determination of Structure of human mitochondrial iron sulfur cluster core complex (NIAUF)2 (PDB ID: 8ZZF, PDB-Dev ID: PDBDEV_00000015)

1. Model Composition	
Entry composition	- Acp: Chain G (70 residues) - Acp: Chain C (71 residues) - PYRIDOXAL-5'-PHOSPHATE: Chain N (Not available residues) - ISCU: Chain D (128 residues) - S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate: Chain L (Not available residues) - NFS1: Chain A (399 residues) - FXN: Chain I (119 residues) - FXN: Chain J (119 residues) - PYRIDOXAL-5'-PHOSPHATE: Chain K (Not available residues) - S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate: Chain O (Not available residues) - ZINC ION: Chain M (Not available residues) - ISD11: Chain F (83 residues) - ZINC ION: Chain P (Not available residues) - ISD11: Chain B (81 residues) - ISCU: Chain H (124 residues) - NFS1: Chain E (401 residues)
Datasets used for modeling	- Experimental model, PDB ID: 5WLW - Experimental model, PDB ID: 1EKG - NMR data, BMRB: 27171 - Crosslinking-MS data, Linker name and number of cross-links: sulfo-SMCC, 1 cross-links - Crosslinking-MS data, Linker name and number of cross-links: sulfo-SMCC, 1 cross-links
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 16
Flexible units	- A: 3-401 - E: 3-403 - I: 1-119 - J: 1-119 - K: None-None - L: None-None - M: None-None - N: None-None - O: None-None - P: None-None - B: 5-85 - C: 4-74 - D: 6-133 - F: 3-85 - G: 3-72 - H: 10-133

Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 2 unique CrossLinkRestraint: sulfo-SMCC, 1 cross-links - 10 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
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 = 17.37, Number of Ramachandran outliers = 18, Number of sidechain outliers = 30
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	None
Name	None
Software	HADDOCK (version 2.2)