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	- NFS1: chain(s) A (406 residues) - ISD11: chain(s) B (91 residues) - Acp: chain(s) C (77 residues) - ISCU: chain(s) D (150 residues) - NFS1: chain(s) E (406 residues) - ISD11: chain(s) F (91 residues) - Acp: chain(s) G (77 residues) - ISCU: chain(s) H (150 residues) - FXN: chain(s) I, J (119 residues) - S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate: chain(s) L [C], O [G] - ZINC ION: chain(s) M [D], P [H]
Datasets used for modeling	- Experimental model, PDB: 5WLW - Experimental model, PDB: 1EKG - NMR data, BMRB: 27171 - Crosslinking-MS data, PRIDE: PXD006938 - Crosslinking-MS data, PRIDE: PXD006928
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 10
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 2 unique CrossLinkRestraint: sulfo-SMCC, 1 crosslinks - 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)	Not available
Data quality	Data quality has not been assessed

Model quality: assessment of atomic segments	- Clashscore: 17.32 - Ramachandran outliers: 18 - Sidechain outliers: 30
Fit to data used for modeling	Satisfaction of crosslinks: 75.00%
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. Name	None
Software	HADDOCK (version 2.2)