Summary of integrative structure determination of structure of human mitochondrial iron sulfur cluster core complex (niauf)2 (PDBDEV00000015)

1. Model Composition	
Entry composition	- ZINC ION: Chain M (None listed residues) - Acp: Chain C (71 residues) - ISD11: Chain B (81 residues) - Acp: Chain G (70 residues) - PYRIDOXAL-5'-PHOSPHATE: Chain K (None listed residues) - S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate: Chain L (None listed residues) - ISD11: Chain F (83 residues) - ZINC ION: Chain P (None listed residues) - NFS1: Chain E (401 residues) - PYRIDOXAL-5'-PHOSPHATE: Chain N (None listed residues) - FXN: Chain J (119 residues) - S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate: Chain O (None listed residues) - ISCU: Chain H (124 residues) - ISCU: Chain D (128 residues) - NFS1: Chain A (399 residues) - FXN: Chain I (119 residues)
Datasets used for modeling	- Experimental model, PDB ID: 5WLW - Experimental model, PDB ID: 1EKG - NMR data, 27171 - CX-MS data, Linker name and number of cross-links: sulfo-SMCC, 1 cross-links - CX-MS data, Linker name and number of cross-links: sulfo-SMCC, 1 cross-links
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	0, 16
Rigid bodies	- A: - - E: - - I: - - J: - - K: - - L: - - M: - - N: - - O: - - P: - - B: - - C: - - D: - - F: - - G: - - H: -

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.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
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	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, Not applicable
Number of ensembles	0
Number of models in ensembles	Not applicable
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Clashscore: 17.02, Ramachandran outliers: 1.14% , Sidechain outliers: 2.67%
Model quality: assessment of excluded volume	- Not applicable
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	None

Name	None
Details	- Method details unspecified
Software	- HADDOCK (version 2.2) - No location specified