Summary of integrative structure determination of Integrative structure of the COX-AIFM1 complex (PDB ID: 9A1K, PDB-Dev ID: PDBDEV_00000092)

1. Model Composition	
Entry composition	- Cytochrome c oxidase polypeptide I: chain(s) A (513 residues) - Cytochrome c oxidase polypeptide II: chain(s) B (226 residues) - Cytochrome c oxidase polypeptide III: chain(s) C (259 residues) - Cytochrome c oxidase subunit IV isoform 1: chain(s) D (144 residues) - Cytochrome c oxidase polypeptide Va: chain(s) E (109 residues) - Cytochrome c oxidase polypeptide Vb: chain(s) F (98 residues) - Cytochrome c oxidase polypeptide VIa-heart: chain(s) G (83 residues) - Cytochrome c oxidase polypeptide VIb: chain(s) H (86 residues) - Cytochrome c oxidase polypeptide VIc: chain(s) I (72 residues) - Cytochrome c oxidase polypeptide VIIa-heart: chain(s) J (58 residues) - Cytochrome c oxidase polypeptide VIIb: chain(s) K (49 residues) - Cytochrome c oxidase polypeptide VIIc: chain(s) L (46 residues) - Cytochrome c oxidase polypeptide VIII-heart: chain(s) M (43 residues) - Cytochrome c oxidase subunit NDUFA4: chain(s) N (80 residues) - Apoptosis inducing factor 1: chain(s) O, P (559 residues)

Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD025102 - Comparative model, Not available - Comparative model, Not available - Comparative model, Not available - Comparative model, Not available - De Novo model, Not available - Experimental model, PDB: 1V54 - Experimental model, PDB: 1OCC - Experimental model, PDB: 2Y69 - Experimental model, PDB: 3J9M - Experimental model, PDB: 4G23 - Experimental model, PDB: 4G26 - Experimental model, PDB: 4LEU - Experimental model, PDB: 5DIZ - Experimental model, PDB: 5FT9 - Experimental model, PDB: 5IWB - Experimental model, PDB: 5ORM - Experimental model, PDB: 5Z62 - Experimental model, PDB: 6F5D - Experimental model, PDB: 6GAW - Experimental model, PDB: 6GAZ - Experimental model, PDB: 6HU9 - Experimental model, PDB: 6LVR - Experimental model, PDB: 2LQT - Experimental model, PDB: 5JJ4 - Experimental model, PDB: 5Z62 - Experimental model, PDB: 6NL3 - Experimental model, PDB: 6PCE - Experimental model, PDB: 6PCF - Experimental model, PDB: 6TDV - Experimental model, PDB: 6X89 - Experimental model, PDB: 4BUR
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 16
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: Other, 1 crosslinks
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: 14.90 - Ramachandran outliers: 61 - Sidechain outliers: 130
Fit to data used for modeling	Satisfaction of crosslinks: 56.52%
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	- trRossetta (version Not available) - Robetta (version Not available) - DisVis (version Not available) - Haddock (version 2.4) - Naccess (version Not available)