

Summary of integrative structure determination of Integrative structure of the COX-AIFM1 complex (PDB ID: 9A1K, PDB-Dev ID: PDBDEV_0000092)

1. Model Composition	
<p>Entry composition</p>	<ul style="list-style-type: none"> - Cytochrome c oxidase polypeptide Va: Chain E (109 residues) - Cytochrome c oxidase polypeptide VIb: Chain H (86 residues) - Apoptosis inducing factor 1: Chain O (559 residues) - Cytochrome c oxidase subunit IV isoform 1: Chain D (144 residues) - Cytochrome c oxidase polypeptide VIc: Chain I (72 residues) - Cytochrome c oxidase polypeptide VIII-heart: Chain M (43 residues) - Cytochrome c oxidase polypeptide VIIc: Chain L (46 residues) - Cytochrome c oxidase subunit NDUFA4: Chain N (80 residues) - Cytochrome c oxidase polypeptide II: Chain B (226 residues) - Apoptosis inducing factor 1: Chain P (559 residues) - Cytochrome c oxidase polypeptide VIIa-heart: Chain J (58 residues) - Cytochrome c oxidase polypeptide III: Chain C (259 residues) - Cytochrome c oxidase polypeptide Vb: Chain F (98 residues) - Cytochrome c oxidase polypeptide VIIb: Chain K (49 residues) - Cytochrome c oxidase polypeptide VIa-heart: Chain G (83 residues) - Cytochrome c oxidase polypeptide I: Chain A (513 residues)

<p><i>Datasets used for modeling</i></p>	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: Other, 1 cross-links - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - De Novo model, Not available - Experimental model, PDB ID: 1V54 - Experimental model, PDB ID: 1OCC - Experimental model, PDB ID: 2Y69 - Experimental model, PDB ID: 3J9M - Experimental model, PDB ID: 4G23 - Experimental model, PDB ID: 4G26 - Experimental model, PDB ID: 4LEU - Experimental model, PDB ID: 5DIZ - Experimental model, PDB ID: 5FT9 - Experimental model, PDB ID: 5IWB - Experimental model, PDB ID: 5ORM - Experimental model, PDB ID: 5Z62 - Experimental model, PDB ID: 6F5D - Experimental model, PDB ID: 6GAW - Experimental model, PDB ID: 6GAZ - Experimental model, PDB ID: 6HU9 - Experimental model, PDB ID: 6LVR - Experimental model, PDB ID: 2LQT - Experimental model, PDB ID: 5JJ4 - Experimental model, PDB ID: 5Z62 - Experimental model, PDB ID: 6NL3 - Experimental model, PDB ID: 6PCE - Experimental model, PDB ID: 6PCF - Experimental model, PDB ID: 6TDV - Experimental model, PDB ID: 6X89 - Experimental model, PDB ID: 4BUR
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of <i>rigid bodies</i>, <i>flexible units</i></i>	0, 16
<i>Flexible units</i>	<ul style="list-style-type: none"> - E: 1-109 - P: 1-559 - H: 1-86 - I: 1-72 - O: 1-559 - N: 1-80 - B: 1-226 - A: 1-513 - C: 1-259 - D: 1-144 - F: 1-98 - G: 1-83 - J: 1-58 - K: 1-49 - L: 1-46 - M: 1-43

Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: Other, 1 cross-links
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: Clashescore = 14.89, Number of Ramachandran outliers = 61, Number of sidechain outliers = 130
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	<ul style="list-style-type: none"> - trRossetta (version Not available) - Robetta (version Not available) - DisVis (version Not available) - Haddock (version 2.4) - Naccess (version Not available)