Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

PDB ID	PDBDEV00000015
Molecule Name	Structure of human mitochondrial iron sulfur cluster core complex (NIAUF)2
Title	Architectural Features of Human Mitochondrial Cysteine Desulfurase Complexes from Crosslinking Mass Spectrometry and Small Angle X-ray Scattering
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The following softwares were used in the production of this report:

Integrative Modeling Package : Version XX
Molprobity : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There is 1 unique type of model in this entry. Model has 16 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	NFS1	A	399
1	ISD11	E	401
1	Acp	B	81
1	ISCU	F	83
1	FXN	C	71
1	PYRIDOXAL-5'-PHOSPHATE	G	70
1	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate	D	128
1	ZINC ION	H	124
1	NFS1	I	119
1	ISD11	J	119

1	Acp	K	None Listed
1	ISCU	N	None Listed
1	FXN	L	None Listed
1	PYRIDOXAL-5'-PHOSPHATE	O	None Listed
1	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate	M	None Listed
1	ZINC ION	P	None Listed

There is 1 software package reported in this entry.

ID	Software Name	Software Version	Software Classification
1	HADDOCK	2.2	molecular docking

There are 5 unique datasets used to build the model in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	5WLW
2	Experimental model	PDB	1EKG
3	NMR data	BMRB	27171
4	CX-MS data	PRIDE	PXD006938
5	CX-MS data	PRIDE	PXD006928

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

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5. Fit of model and data

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6. Uncertaintiy of model