

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 06:51 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 |
| Authors | Cai K;Frederick RO;Dashti H;Markley JL |

The following softwares were used in the production of this report:

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

1. Overall quality at a glance

2. Entry composition

There are 2 unique types of models in this entry. This entry contains 16 unique chains.

| 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-(phosphonoxy)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

5. Fit of model and data

6. Uncertainty of model
