Full wwPDB Integrative Structure Validation Report

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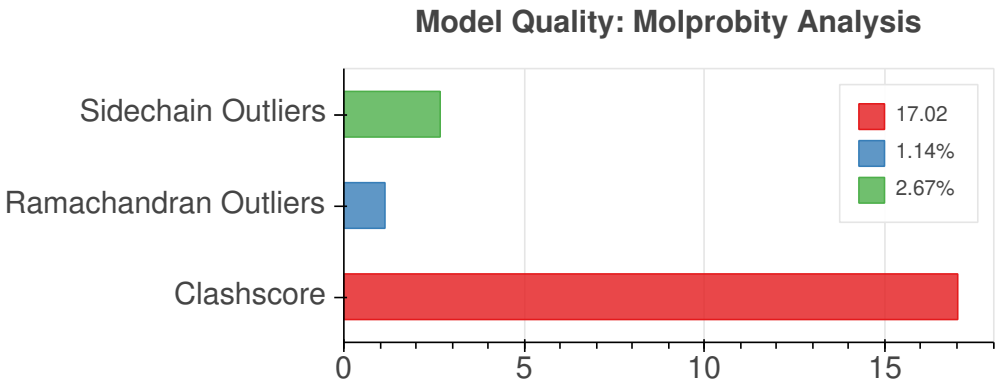
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 16 subunits in each model. A total of 5 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 16 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled None/Best Scoring Model respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	NFS1	A	399
1	2	1	NFS1	E	401
1	3	2	ISD11	B	81
1	4	2	ISD11	F	83
1	5	3	Acp	C	71
1	6	3	Acp	G	70
1	7	4	ISCU	D	128
1	8	4	ISCU	H	124
1	9	5	FXN	I	119
1	10	5	FXN	J	119
1	11	6	PYRIDOXAL-5'-PHOSPHATE	K	None listed
1	12	6	PYRIDOXAL-5'-PHOSPHATE	N	None listed
1	13	7	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-L-beta-alanyl}amino)ethyl] dodecanethioate		None listed

1	14	7	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]beta-alanyl}amino)ethyl] dodecanethioate	O	None listed
1	15	8	ZINC ION	M	None listed
1	16	8	ZINC ION	P	None listed

3.3 Datasets used for modeling

There are 5 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 0 rigid bodies and 16 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	-	3-401.
B	-	5-85.
C	-	4-74.
D	-	6-133.
E	-	3-403.
F	-	3-85.
G	-	3-72.
H	-	10-133.

I	-	1-119.
J	-	1-119.
K	-	None-None.
L	-	None-None.
M	-	None-None.
N	-	None-None.
O	-	None-None.
P	-	None-None.

5. Methodology and software

There is 1 software package reported in this entry.

ID	*Software name*	*Software version*	*Software classification*
1	HADDOCK	2.2	molecular docking

6. Data quality

7. Model quality

7.1 Standard geometry

There are 397 bond outliers in this entry.

Bond type	*Observed distance (Å)*	*Ideal distance (Å)*	*Number of outliers*
C6--H6	0.93	1.09	0
NZ--HZ3	1.039	0.89	19
NH2--HH21	1.004	0.86	3
NZ--HZ2	1.038	0.89	19
NZ--HZ1	1.038	0.89	19

NH1--HH11	1.004	0.86	3
NH1--HH12	1.003	0.86	3
NH2--HH22	1	0.86	3
OH--HH	0.962	0.84	13
OG1--HG1	0.965	0.84	19
OG--HG	0.964	0.84	23
NE2--HE21	0.98	0.86	3
N--H	0.977	0.86	227
NE--HE	0.985	0.86	3
ND2--HD21	0.979	0.86	5
NE1--HE1	0.982	0.86	5
ND2--HD22	0.981	0.86	5
NE2--HE2	0.981	0.86	3
NE2--HE22	0.98	0.86	3

There are 0 angle outliers in this entry.

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	***Clash score***	***Number of clashes***
Model 1	17.02	388

All 388 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	***Analyzed***	***Favored***	***Allowed***	***Outliers***

1	1575	1503	54	18

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:273	ARG
1	A:275	ARG
1	A:381	CYS
1	A:447	ILE
1	C:72	ILE
1	D:7	SER
1	D:8	VAL
1	D:32	LYS
1	D:42	PRO
1	D:45	GLY
1	E:273	ARG
1	E:274	PRO
1	E:384	ALA
1	E:386	LEU
1	H:18	TYR
1	H:20	ASN
1	H:42	PRO
1	H:85	LYS

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	1124	1010	84	30

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:172	GLN
1	A:272	ARG
1	A:277	ARG
1	B:65	VAL
1	C:10	ILE
1	C:36	SER
1	C:52	THR
1	E:143	ARG
1	E:172	GLN
1	F:61	ARG
1	G:20	GLU
1	G:36	SER
1	H:13	GLN
1	H:60	ILE
1	H:77	SER
1	H:133	GLU
1	I:91	ASP
1	I:93	THR
1	I:113	LEU
1	I:119	THR
1	I:133	THR
1	I:139	ASP
1	I:144	VAL
1	J:91	ASP
1	J:93	THR

1	J:113	LEU
1	J:119	THR
1	J:133	THR
1	J:139	ASP
1	J:144	VAL

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model