Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 08:57 PM

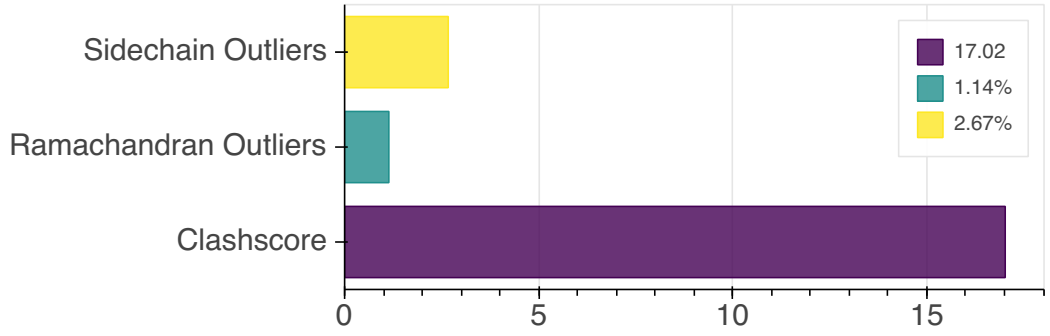
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000015
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

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

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.

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	13	7	S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate	L	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

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	None	False	None

Data quality

Model quality

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

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
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	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.

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.

Torsion angles: Protein backbone

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

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

Torsion angles: 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

Model ID	Chain and res ID	Residue type
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

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model