

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

PDB ID	PDBDEV00000002
Molecule Name	Structure of Saccharomyces cerevisiae exosome determined with CX-MS
Title	A strategy for dissecting the architectures of native macromolecular assemblies.
Authors	Shi Y;Pellarin R;Fridy PC;Fernandez-Martinez J;Thompson MK;Li Y;Wang QJ;Sali A;Rout MP;Chait B

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 are 1 unique types of models in this entry. The entry contains 38 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Dis3	Α	1001
1	Rrp45	В	305
1	Rrp4	С	359
1	Csl4	D	292
1	Mtr3	E	250
1	Rrp40	F	240
1	Rrp42	G	265
1	Ski6	Н	265
1	Rrp46_gfp	1	475
1	Rrp43	J	394
1	Lrp1	К	184
1	Rrn6	ı	733

•	11100	_	,
1	MPP6	М	186
1	RPL3	N	747

There are 3 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building
2	IMP PMI module	67456c0	integrative model building
3	Phyre2	2.0	protein homology modeling

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

ID	Dataset Type	Database Name	Data Access Code
1	Experimental model	PDB	4IFD
2	Experimental model	PDB	1GFL
3	Experimental model	PDB	2HBJ
4	Comparative model	Not Listed	None
5	CX-MS data	Not Listed	None

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.2 Protein sidechains		
5. Fit of model and data		
6. Uncertaintiy of model		

4.2.1 Protein backbone