

PDB

# Full RCSB Integrative Structure Validation Report

July 09, 2021 -- 12:20 PM

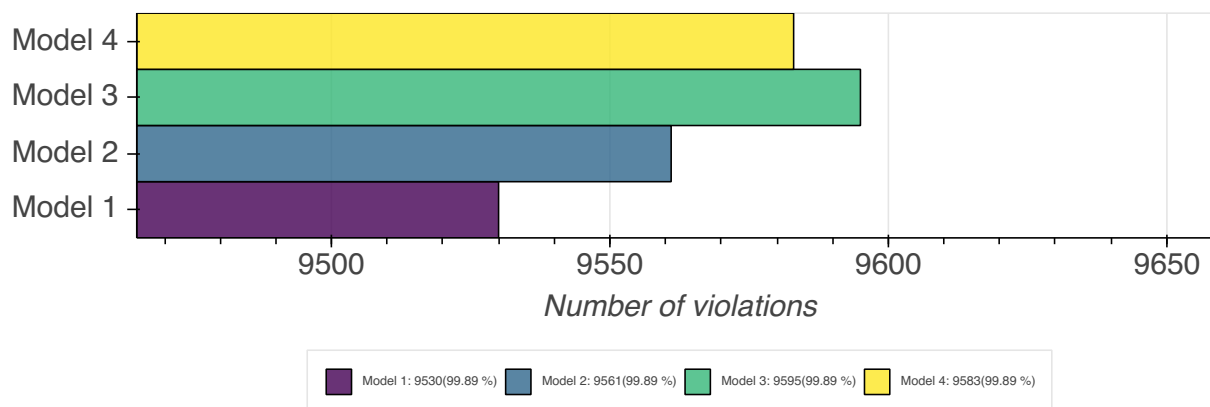
The following software were used in the production of this report:

*Integrative Modeling Validation Package : Version 1.0*

PDB ID	PDBDEV_00000002
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 BT

## Overall quality

### Model quality: Excluded Volume Analysis



### Ensemble information

*This entry consists of 4 distinct ensembles.*

### Entry composition

*There are 4 unique types of models in this entry. These models are titled Rrp6 cluster 1/Best scoring model, Rrp6 cluster 2/Best scoring model, Ski7 cluster 1/Best scoring model, Ski7 cluster 2/Best scoring model respectively.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	Dis3	A	1001
1	2	2	Rrp45	B	305
1	3	3	Rrp4	C	359
1	4	4	Csl4	D	292
1	5	5	Mtr3	E	250
1	6	6	Rrp40	F	240
1	7	7	Rrp42	G	265
1	8	8	Ski6	H	265
1	9	9	Rrp46_gfp	I	475
1	10	10	Rrp43	J	394
1	11	11	Lrp1	K	184
1	12	12	Rrp6	L	733
1	13	13	MPP6	M	186
2	1	1	Dis3	A	1001
2	2	2	Rrp45	B	305
2	3	3	Rrp4	C	359

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
2	4	4	Csl4	D	292
2	5	5	Mtr3	E	250
2	6	6	Rrp40	F	240
2	7	7	Rrp42	G	265
2	8	8	Ski6	H	265
2	9	9	Rrp46_gfp	I	475
2	10	10	Rrp43	J	394
2	11	11	Lrp1	K	184
2	12	12	Rrp6	L	733
2	13	13	MPP6	M	186
3	1	1	Dis3	A	1001
3	2	2	Rrp45	B	305
3	3	3	Rrp4	C	359
3	4	4	Csl4	D	292
3	5	5	Mtr3	E	250
3	6	6	Rrp40	F	240
3	7	7	Rrp42	G	265
3	8	8	Ski6	H	265
3	9	9	Rrp46_gfp	I	475
3	10	10	Rrp43	J	394
3	11	15	Ski7	N	747
4	1	1	Dis3	A	1001
4	2	2	Rrp45	B	305

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
4	3	3	Rrp4	C	359
4	4	4	Csl4	D	292
4	5	5	Mtr3	E	250
4	6	6	Rrp40	F	240
4	7	7	Rrp42	G	265
4	8	8	Ski6	H	265
4	9	9	Rrp46_gfp	I	475
4	10	10	Rrp43	J	394
4	11	15	Ski7	N	747

### Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	50000	True	True
1	2	Replica exchange monte carlo	Sampling	50000	True	True

### Data quality

#### Model quality

##### Excluded volume satisfaction

*Excluded volume satisfaction for the models in the entry are listed below.*

Models	Excluded Volume Satisfaction	Number of violations
1	99.89	9530.0
2	99.89	9561.0
3	99.89	9595.0
4	99.89	9583.0

---

Fit of model to data used for modeling

---

Fit of model to data not used for modeling

---

Uncertainty of data and model