



Full wwPDB Integrative Structure Validation Report

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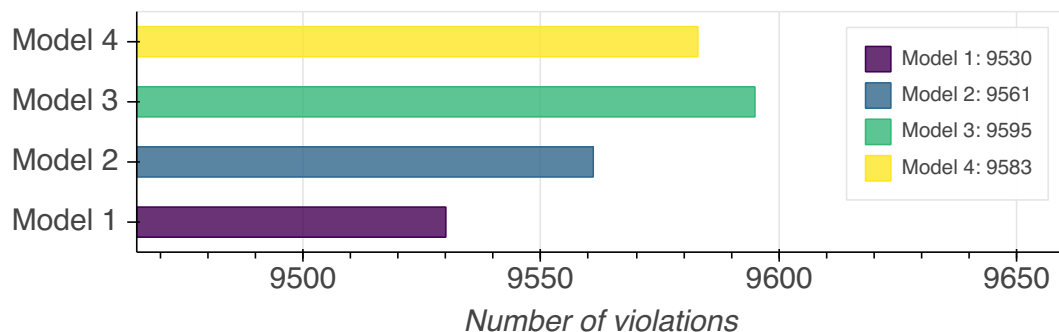
The following software were used in the production of this report:

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	False	True
1	2	Replica exchange monte carlo	Sampling	50000	False	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