Integrative Structure Validation Report July 22, 2024 - 03:30 PM PDT

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

Python-IHM Version 1.3 Integrative Modeling Validation Version 1.2

PDB ID	8ZZ2
PDB-Dev ID	PDBDEV_00000002
Structure Title	Structure of Saccharomyces cerevisiae exosome determined with CX-MS
Structure Authors	Shi Y; Pellarin R; Fridy PC; Fernandez-Martinez J; Thompson MK; Li Y; Wang QJ; Sali A; Rout MP; Chait BT

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

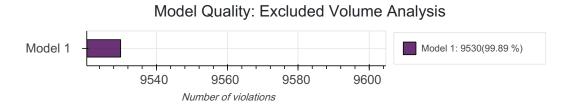
We welcome your comments at pdb-dev@mail.wwpdb.org

A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

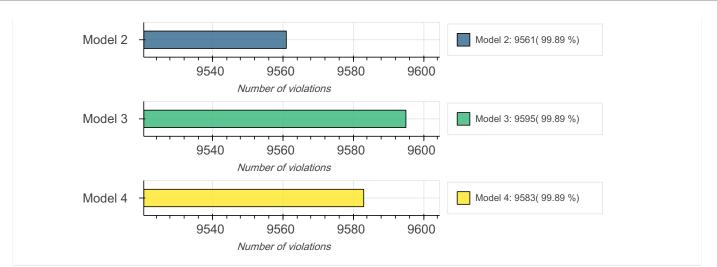
Overall quality o

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.



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This entry consists of 4 distinct ensemble(s).

Summary ?

This entry consists of 4 unique models, with 12 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 30 rigid bodies and 31 flexible or non-rigid units.

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	Chain ID [auth]	Total residues
1	1	1	Dis3	А	А	1001
1	2	2	Rrp45	В	В	305
1	3	3	Rrp4	С	С	359
1	4	4	Csl4	D	D	292
1	5	5	Mtr3	E	E	250
1	6	6	Rrp40	F	F	240
1	7	7	Rrp42	G	G	265

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	8	8	Ski6	Н	Н	265
1	9	9	Rrp46_gfp	I	I	475
1	10	10	Rrp43	J	J	394
1	11	11	Lrp1	К	к	184
1	12	12	Rrp6	L	L	733
1	13	13	MPP6	М	М	186
2	1	1	Dis3	А	А	1001
2	2	2	Rrp45	В	В	305
2	3	3	Rrp4	С	С	359
2	4	4	Csl4	D	D	292
2	5	5	Mtr3	E	E	250
2	6	6	Rrp40	F	F	240
2	7	7	Rrp42	G	G	265
2	8	8	Ski6	Н	Н	265
2	9	9	Rrp46_gfp	I	I	475
2	10	10	Rrp43	J	J	394
2	11	11	Lrp1	К	К	184
2	12	12	Rrp6	L	L	733
2	13	13	MPP6	М	М	186
3	1	1	Dis3	А	А	1001
3	2	2	Rrp45	В	В	305
3	3	3	Rrp4	С	С	359
3	4	4	Csl4	D	D	292

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	5	5	Mtr3	E	E	250
3	6	6	Rrp40	F	F	240
3	7	7	Rrp42	G	G	265
3	8	8	Ski6	Н	Н	265
3	9	9	Rrp46_gfp	I	I	475
3	10	10	Rrp43	J	J	394
3	11	15	Ski7	Ν	Ν	747
4	1	1	Dis3	А	А	1001
4	2	2	Rrp45	В	В	305
4	3	3	Rrp4	С	С	359
4	4	4	Csl4	D	D	292
4	5	5	Mtr3	E	E	250
4	6	6	Rrp40	F	F	240
4	7	7	Rrp42	G	G	265
4	8	8	Ski6	Н	Н	265
4	9	9	Rrp46_gfp	I	I	475
4	10	10	Rrp43	J	J	394
4	11	15	Ski7	Ν	Ν	747

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	4IFD

ID	Dataset type	Database name	Data access code
2	Experimental model	PDB	1GFL
3	Experimental model	PDB	2HBJ
4	Comparative model	File	10.5281/zenodo.583313
5	Crosslinking-MS data	File	10.5281/zenodo.583313

Representation ?

This entry has only one representation and includes 30 rigid bodies and 31 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	9-237, 249-329, 364-471, 472-1001	1-8, 238-248, 330-363
В	2-301	1-1, 302-305
С	2-17, 50-102, 103-245, 275-357	1-1, 18-49, 246-274, 358-359
D	1-71, 99-113, 126-162, 185-291	72-98, 114-125, 163-184, 292-292
E	4-22, 42-149, 163-248	1-3, 23-41, 150-162, 249-250
F	1-60, 61-236	237-240
G	1-265	-
н	1-242	243-265
I	1-223, 247-475	224-246
J	7-99, 121-193, 206-309, 327-394	1-6, 100-120, 194-205, 310-326
к	-	1-184
L	127-516, 532-557, 565-619	1-126, 517-531, 558-564, 620-733
М	-	1-186
Ν	259-747	1-258

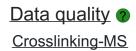
Methodology and software

This entry is a result of 2 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	50000	True	True
1	2	Replica exchange monte carlo	Sampling	None	50000	True	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop- 0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	Phyre2	2.0	protein homology modeling	http://www.sbg.bio.ic.ac.uk/~phyre2/



Validation for this section is under development.

	Model quality	
	tomic structures, molprobity analysis is performed. For mode ed volume analysis is performed.	els with coarse-grained or multi-scale
	me satisfaction ? satisfaction for the models in the entry are listed below.	
Models	Excluded Volume Satisfaction (%)	Number of violations

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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 @

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

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