WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB Integrative Structure Validation Report

November 07, 2019 -- 03:35 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 BT

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

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

Model quality: Excluded Volume Analysis
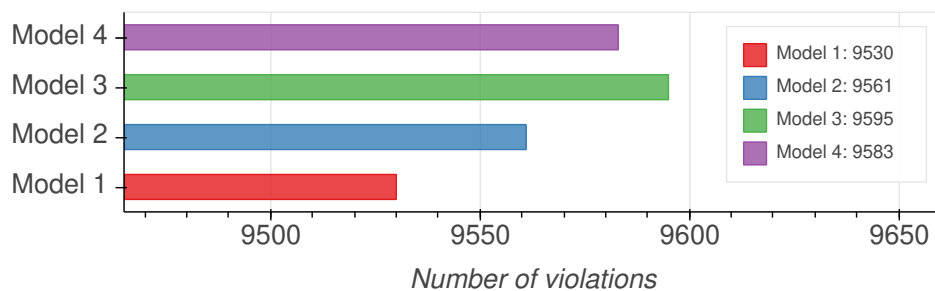
2. Ensemble information

This entry consists of 4 distinct ensembles.

Ensemble number	Ensemble name	Model ID	Number of models	Clustering method	Clustering feature	Cluster precision
1	Rrp6 cluster 1	1	69	None	RMSD	24.374
2	Rrp6 cluster 2	2	131	None	RMSD	19.258

| 3 | Ski7 cluster 1 | 3 | 159 | None | RMSD | 9.798 |
| 4 | Ski7 cluster 2 | 4 | 41 | None | RMSD | 11.517 |

3. Model composition

3.1 Summary

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

3.2 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
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
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

3.3 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
2	Experimental model	PDB	1GFL
3	Experimental model	PDB	2HBJ
4	Comparative model	Not listed	None
5	CX-MS data	Not listed	None

4. 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:Experimental model/4IFD, 249-329:Experimental model/4IFD, 364-471:Experimental model/4IFD, 472-1001:Experimental model/4IFD.	1-8, 238-248, 330-363.
B	2-301:Experimental model/4IFD.	1-1, 302-305.
C	2-17:Experimental model/4IFD, 50-102:Experimental model/4IFD, 103-245:Experimental model/4IFD, 275-357:Experimental model/4IFD.	1-1, 18-49, 246-274, 358-359.
D	1-71:Experimental model/4IFD, 99-113:Experimental model/4IFD, 126-162:Experimental model/4IFD, 185-291:Experimental model/4IFD.	72-98, 114-125, 163-184, 292-292.
E	4-22:Experimental model/4IFD, 42-149:Experimental model/4IFD, 163-248:Experimental model/4IFD.	1-3, 23-41, 150-162, 249-250.
F	1-60:Experimental model/4IFD, 61-236:Experimental model/4IFD.	237-240.
G	1-265:Experimental model/4IFD.	-
H	1-242:Experimental model/4IFD.	243-265.
I	1-223:Experimental model/4IFD, 247-475:Experimental model/1GFL.	224-246.

J	7-99:Experimental model/4IFD, 121-193:Experimental model/4IFD, 206-309:Experimental model/4IFD, 327-394:Experimental model/4IFD.	1-6, 100-120, 194-205, 310-326.
K	-	1-184.
L	127-516:Experimental model/2HBJ, 532-557:Experimental model/4IFD, 565-619:Experimental model/4IFD.	1-126, 517-531, 558-564, 620-733.
M	-	1-186.
N	259-747:Comparative model/None.	1-258.

5. 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

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.or
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.or
3	Phyre2	2.0	protein homology modeling	http://www.sbg.bio.ic.ac.uk/~p

6. Data quality

7. Model quality

7.1 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

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model