Full wwPDB Integrative Structure Validation Report

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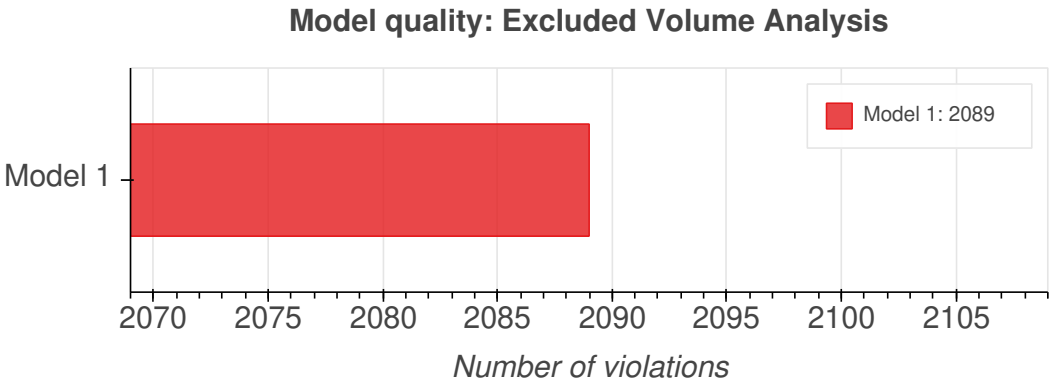
PDB ID	***PDBDEV00000017***
Molecule Name	Molecular architecture of the major membrane ring component, Pom152, of the yeast nuclear pore complex
Title	Molecular Architecture of the Major Membrane Ring Component of the Nuclear Pore Complex.
Authors	Upla P;Kim SJ;Sampathkumar P;Dutta K;Cahill SM;Chemmama IE;Williams R;Bonanno JB;Rice WJ;Stokes DL;Cowburn D;Almo SC;Sali A;Rout MP;Fernandez-Martinez J

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

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 1 distinct ensemble.

Ensemble number	Ensemble name	Model ID	Number of models	Clustering method	Clustering feature	Cluster precision
1	Cluster 0	1	364	None	dRMSD	7.0

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 1 subunits in each model. A total of 22 datasets or restraints was used to build this entry. Each model is represented by 9 rigid bodies and 9 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled Cluster 0/None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	pom152	A	1337

3.3 Datasets used for modeling

There are 22 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5TVZ
2	Comparative model	Not listed	None
3	Comparative model	Not listed	None
4	Comparative model	Not listed	None
5	Comparative model	Not listed	None
6	Comparative model	Not listed	None
7	Comparative model	Not listed	None
8	3DEM volume	EMDB	EMD-8543
9	3DEM volume	Not listed	None
10	2DEM class average	Not listed	None
11	2DEM class average	Not listed	None
12	2DEM class average	Not listed	None

13	2DEM class average	Not listed	None
14	2DEM class average	Not listed	None
15	2DEM class average	Not listed	None
16	2DEM class average	Not listed	None
17	2DEM class average	Not listed	None
18	SAS data	SASBDB	SASDBV9
19	SAS data	SASBDB	SASDBW9
20	SAS data	SASBDB	SASDBX9
21	SAS data	SASBDB	SASDBY9
22	SAS data	SASBDB	SASDBZ9

4. Representation

This entry has only one representation and includes 9 rigid bodies and 9 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	379-472:Comparative model/None, 520-611:Comparative model/None, 616-714:Comparative model/None, 722-818:Comparative model/None, 824-918:Comparative model/None, 931-1026:Comparative model/None, 1036-1141:Comparative model/None, 1150-1229:Comparative model/None, 1244-1337:Comparative model/None.	1-378, 473-519, 612-615, 715-721, 819-823, 919-930, 1027-1035, 1142-1149, 1230-1243.

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	100000	False	True

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	MODELLER	9.13	comparative modeling

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	99.46	2089

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model