

Integrative Structure Validation Report ?

July 22, 2024 - 04:41 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	9A1P
PDB-Dev ID	PDBDEV_00000097
Structure Title	Comprehensive structure and functional adaptations of the yeast nuclear pore complex
Structure Authors	Akey CW; Singh D; Ouch C; Echeverria I; Nudelman I; Varberg JM; Yu Z; Fang F; Shi Y; Wang J; Salzberg D; Song K; Xu C; Gumbart JC; Suslov S; Unruh J; Jaspersen SL; Chait BT; Sali A; Fernandez-Martinez J; Ludtke SJ; Villa E; Rout MP

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

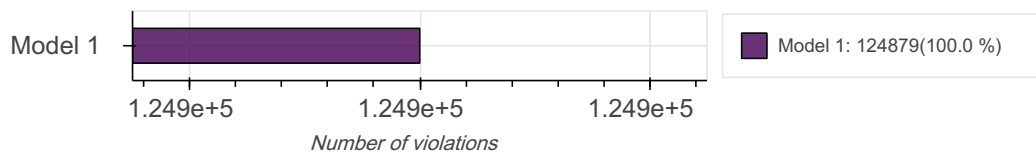
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

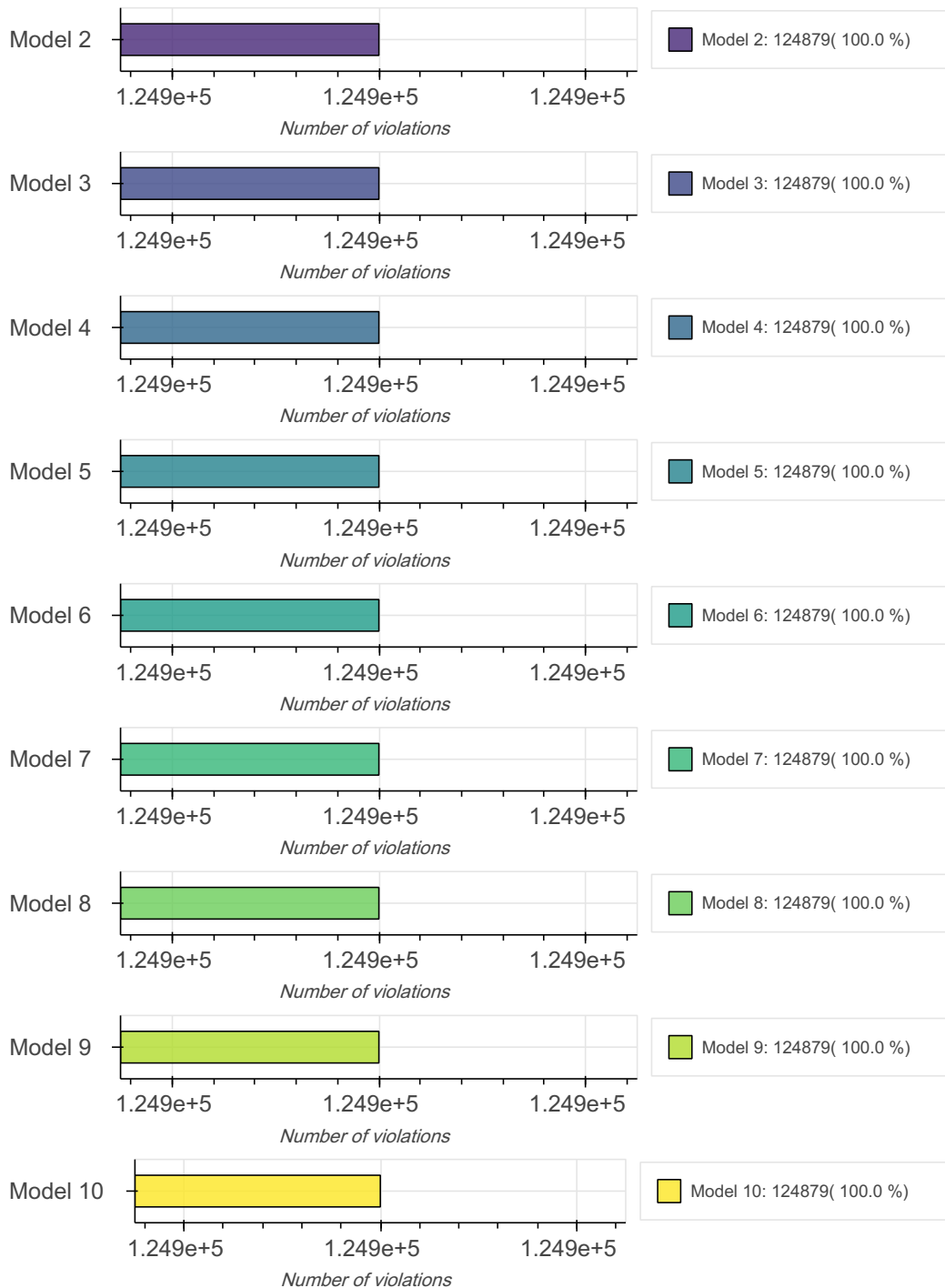
List of references used to build this report is available [here](#).

Overall quality ?

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.

Model Quality: Excluded Volume Analysis





Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 10 unique models, with 28 subunits in each model. A total of 3 datasets or restraints were used to build this entry. Each model is represented by 28 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There are 10 unique types of models in this entry. These models are titled Model 1, Model 2, Model 3, Model 4, Model 5, Model 6, Model 7, Model 8, Model 9, Model 10 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Nup157	Z	Z	1391
1	2	1	Nup157	1	1	1391
1	3	2	Nup170	Y	Y	1502
1	4	2	Nup170	0	0	1502
1	5	3	Nup53	U	U	475
1	6	3	Nup53	W	W	475
1	7	4	Nup59	V	V	528
1	8	4	Nup59	X	X	528
1	9	5	Nsp1	A	A	823
1	10	5	Nsp1	D	D	823
1	11	5	Nsp1	G	G	823
1	12	5	Nsp1	J	J	823
1	13	6	Nup57	B	B	541
1	14	6	Nup57	E	E	541
1	15	6	Nup57	H	H	541
1	16	6	Nup57	K	K	541
1	17	7	Nup49	C	C	472
1	18	7	Nup49	F	F	472
1	19	7	Nup49	I	I	472
1	20	7	Nup49	L	L	472

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	21	8	Nup188	N	N	1655
1	22	8	Nup188	P	P	1655
1	23	9	Nup192	M	M	1683
1	24	9	Nup192	O	O	1683
1	25	10	Nic96	Q	Q	839
1	26	10	Nic96	R	R	839
1	27	10	Nic96	S	S	839
1	28	10	Nic96	T	T	839
2	1	1	Nup157	Z	Z	1391
2	2	1	Nup157	1	1	1391
2	3	2	Nup170	Y	Y	1502
2	4	2	Nup170	0	0	1502
2	5	3	Nup53	U	U	475
2	6	3	Nup53	W	W	475
2	7	4	Nup59	V	V	528
2	8	4	Nup59	X	X	528
2	9	5	Nsp1	A	A	823
2	10	5	Nsp1	D	D	823
2	11	5	Nsp1	G	G	823
2	12	5	Nsp1	J	J	823
2	13	6	Nup57	B	B	541
2	14	6	Nup57	E	E	541
2	15	6	Nup57	H	H	541

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	16	6	Nup57	K	K	541
2	17	7	Nup49	C	C	472
2	18	7	Nup49	F	F	472
2	19	7	Nup49	I	I	472
2	20	7	Nup49	L	L	472
2	21	8	Nup188	N	N	1655
2	22	8	Nup188	P	P	1655
2	23	9	Nup192	M	M	1683
2	24	9	Nup192	O	O	1683
2	25	10	Nic96	Q	Q	839
2	26	10	Nic96	R	R	839
2	27	10	Nic96	S	S	839
2	28	10	Nic96	T	T	839
3	1	1	Nup157	Z	Z	1391
3	2	1	Nup157	1	1	1391
3	3	2	Nup170	Y	Y	1502
3	4	2	Nup170	0	0	1502
3	5	3	Nup53	U	U	475
3	6	3	Nup53	W	W	475
3	7	4	Nup59	V	V	528
3	8	4	Nup59	X	X	528
3	9	5	Nsp1	A	A	823

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
3	10	5	Nsp1	D	D	823
3	11	5	Nsp1	G	G	823
3	12	5	Nsp1	J	J	823
3	13	6	Nup57	B	B	541
3	14	6	Nup57	E	E	541
3	15	6	Nup57	H	H	541
3	16	6	Nup57	K	K	541
3	17	7	Nup49	C	C	472
3	18	7	Nup49	F	F	472
3	19	7	Nup49	I	I	472
3	20	7	Nup49	L	L	472
3	21	8	Nup188	N	N	1655
3	22	8	Nup188	P	P	1655
3	23	9	Nup192	M	M	1683
3	24	9	Nup192	O	O	1683
3	25	10	Nic96	Q	Q	839
3	26	10	Nic96	R	R	839
3	27	10	Nic96	S	S	839
3	28	10	Nic96	T	T	839
4	1	1	Nup157	Z	Z	1391
4	2	1	Nup157	1	1	1391
4	3	2	Nup170	Y	Y	1502
4	4	2	Nup170	0	0	1502

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	5	3	Nup53	U	U	475
4	6	3	Nup53	W	W	475
4	7	4	Nup59	V	V	528
4	8	4	Nup59	X	X	528
4	9	5	Nsp1	A	A	823
4	10	5	Nsp1	D	D	823
4	11	5	Nsp1	G	G	823
4	12	5	Nsp1	J	J	823
4	13	6	Nup57	B	B	541
4	14	6	Nup57	E	E	541
4	15	6	Nup57	H	H	541
4	16	6	Nup57	K	K	541
4	17	7	Nup49	C	C	472
4	18	7	Nup49	F	F	472
4	19	7	Nup49	I	I	472
4	20	7	Nup49	L	L	472
4	21	8	Nup188	N	N	1655
4	22	8	Nup188	P	P	1655
4	23	9	Nup192	M	M	1683
4	24	9	Nup192	O	O	1683
4	25	10	Nic96	Q	Q	839
4	26	10	Nic96	R	R	839
4	27	10	Nic96	S	S	839

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	28	10	Nic96	T	T	839
5	1	1	Nup157	Z	Z	1391
5	2	1	Nup157	1	1	1391
5	3	2	Nup170	Y	Y	1502
5	4	2	Nup170	0	0	1502
5	5	3	Nup53	U	U	475
5	6	3	Nup53	W	W	475
5	7	4	Nup59	V	V	528
5	8	4	Nup59	X	X	528
5	9	5	Nsp1	A	A	823
5	10	5	Nsp1	D	D	823
5	11	5	Nsp1	G	G	823
5	12	5	Nsp1	J	J	823
5	13	6	Nup57	B	B	541
5	14	6	Nup57	E	E	541
5	15	6	Nup57	H	H	541
5	16	6	Nup57	K	K	541
5	17	7	Nup49	C	C	472
5	18	7	Nup49	F	F	472
5	19	7	Nup49	I	I	472
5	20	7	Nup49	L	L	472
5	21	8	Nup188	N	N	1655
5	22	8	Nup188	P	P	1655

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
5	23	9	Nup192	M	M	1683
5	24	9	Nup192	O	O	1683
5	25	10	Nic96	Q	Q	839
5	26	10	Nic96	R	R	839
5	27	10	Nic96	S	S	839
5	28	10	Nic96	T	T	839
6	1	1	Nup157	Z	Z	1391
6	2	1	Nup157	1	1	1391
6	3	2	Nup170	Y	Y	1502
6	4	2	Nup170	0	0	1502
6	5	3	Nup53	U	U	475
6	6	3	Nup53	W	W	475
6	7	4	Nup59	V	V	528
6	8	4	Nup59	X	X	528
6	9	5	Nsp1	A	A	823
6	10	5	Nsp1	D	D	823
6	11	5	Nsp1	G	G	823
6	12	5	Nsp1	J	J	823
6	13	6	Nup57	B	B	541
6	14	6	Nup57	E	E	541
6	15	6	Nup57	H	H	541
6	16	6	Nup57	K	K	541

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	17	7	Nup49	C	C	472
6	18	7	Nup49	F	F	472
6	19	7	Nup49	I	I	472
6	20	7	Nup49	L	L	472
6	21	8	Nup188	N	N	1655
6	22	8	Nup188	P	P	1655
6	23	9	Nup192	M	M	1683
6	24	9	Nup192	O	O	1683
6	25	10	Nic96	Q	Q	839
6	26	10	Nic96	R	R	839
6	27	10	Nic96	S	S	839
6	28	10	Nic96	T	T	839
7	1	1	Nup157	Z	Z	1391
7	2	1	Nup157	1	1	1391
7	3	2	Nup170	Y	Y	1502
7	4	2	Nup170	0	0	1502
7	5	3	Nup53	U	U	475
7	6	3	Nup53	W	W	475
7	7	4	Nup59	V	V	528
7	8	4	Nup59	X	X	528
7	9	5	Nsp1	A	A	823
7	10	5	Nsp1	D	D	823
7	11	5	Nsp1	G	G	823

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
7	12	5	Nsp1	J	J	823
7	13	6	Nup57	B	B	541
7	14	6	Nup57	E	E	541
7	15	6	Nup57	H	H	541
7	16	6	Nup57	K	K	541
7	17	7	Nup49	C	C	472
7	18	7	Nup49	F	F	472
7	19	7	Nup49	I	I	472
7	20	7	Nup49	L	L	472
7	21	8	Nup188	N	N	1655
7	22	8	Nup188	P	P	1655
7	23	9	Nup192	M	M	1683
7	24	9	Nup192	O	O	1683
7	25	10	Nic96	Q	Q	839
7	26	10	Nic96	R	R	839
7	27	10	Nic96	S	S	839
7	28	10	Nic96	T	T	839
8	1	1	Nup157	Z	Z	1391
8	2	1	Nup157	1	1	1391
8	3	2	Nup170	Y	Y	1502
8	4	2	Nup170	0	0	1502
8	5	3	Nup53	U	U	475
8	6	3	Nup53	W	W	475

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
8	7	4	Nup59	V	V	528
8	8	4	Nup59	X	X	528
8	9	5	Nsp1	A	A	823
8	10	5	Nsp1	D	D	823
8	11	5	Nsp1	G	G	823
8	12	5	Nsp1	J	J	823
8	13	6	Nup57	B	B	541
8	14	6	Nup57	E	E	541
8	15	6	Nup57	H	H	541
8	16	6	Nup57	K	K	541
8	17	7	Nup49	C	C	472
8	18	7	Nup49	F	F	472
8	19	7	Nup49	I	I	472
8	20	7	Nup49	L	L	472
8	21	8	Nup188	N	N	1655
8	22	8	Nup188	P	P	1655
8	23	9	Nup192	M	M	1683
8	24	9	Nup192	O	O	1683
8	25	10	Nic96	Q	Q	839
8	26	10	Nic96	R	R	839
8	27	10	Nic96	S	S	839
8	28	10	Nic96	T	T	839
9	1	1	Nup157	Z	Z	1391

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	2	1	Nup157	1	1	1391
9	3	2	Nup170	Y	Y	1502
9	4	2	Nup170	0	0	1502
9	5	3	Nup53	U	U	475
9	6	3	Nup53	W	W	475
9	7	4	Nup59	V	V	528
9	8	4	Nup59	X	X	528
9	9	5	Nsp1	A	A	823
9	10	5	Nsp1	D	D	823
9	11	5	Nsp1	G	G	823
9	12	5	Nsp1	J	J	823
9	13	6	Nup57	B	B	541
9	14	6	Nup57	E	E	541
9	15	6	Nup57	H	H	541
9	16	6	Nup57	K	K	541
9	17	7	Nup49	C	C	472
9	18	7	Nup49	F	F	472
9	19	7	Nup49	I	I	472
9	20	7	Nup49	L	L	472
9	21	8	Nup188	N	N	1655
9	22	8	Nup188	P	P	1655
9	23	9	Nup192	M	M	1683

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
9	24	9	Nup192	O	O	1683
9	25	10	Nic96	Q	Q	839
9	26	10	Nic96	R	R	839
9	27	10	Nic96	S	S	839
9	28	10	Nic96	T	T	839
10	1	1	Nup157	Z	Z	1391
10	2	1	Nup157	1	1	1391
10	3	2	Nup170	Y	Y	1502
10	4	2	Nup170	0	0	1502
10	5	3	Nup53	U	U	475
10	6	3	Nup53	W	W	475
10	7	4	Nup59	V	V	528
10	8	4	Nup59	X	X	528
10	9	5	Nsp1	A	A	823
10	10	5	Nsp1	D	D	823
10	11	5	Nsp1	G	G	823
10	12	5	Nsp1	J	J	823
10	13	6	Nup57	B	B	541
10	14	6	Nup57	E	E	541
10	15	6	Nup57	H	H	541
10	16	6	Nup57	K	K	541
10	17	7	Nup49	C	C	472
10	18	7	Nup49	F	F	472

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
10	19	7	Nup49	I	I	472
10	20	7	Nup49	L	L	472
10	21	8	Nup188	N	N	1655
10	22	8	Nup188	P	P	1655
10	23	9	Nup192	M	M	1683
10	24	9	Nup192	O	O	1683
10	25	10	Nic96	Q	Q	839
10	26	10	Nic96	R	R	839
10	27	10	Nic96	S	S	839
10	28	10	Nic96	T	T	839

Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	File	10.5281/zenodo.5662389
2	3DEM volume	EMDB	EMDB-24232
3	Experimental model	PDB	7N85

Representation

This entry has only one representation and includes 28 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
Z	1-1391	-

Chain ID	Rigid bodies	Non-rigid segments
1	1-1391	-
Y	1-1502	-
0	1-1502	-
U	1-475	-
W	1-475	-
V	1-528	-
X	1-528	-
A	1-823	-
D	1-823	-
G	1-823	-
J	1-823	-
B	1-541	-
E	1-541	-
H	1-541	-
K	1-541	-
C	1-472	-
F	1-472	-
I	1-472	-
L	1-472	-
N	1-1655	-
P	1-1655	-
M	1-1683	-
O	1-1683	-

Chain ID	Rigid bodies	Non-rigid segments
Q	1-839	-
R	1-839	-
S	1-839	-
T	1-839	-

Methodology and software ?

This entry is a result of 1 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	Enumeration	Production sampling	None	1200	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	PSIPRED	4.0	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
2	Integrative Modeling Platform (IMP)	2.2	integrative model building	https://integrativemodeling.org

Data quality ?

3DEM volume

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobtity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

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

Models	Excluded Volume Satisfaction (%)	Number of violations
1	100.0	124879.0
2	100.0	124879.0
3	100.0	124879.0
4	100.0	124879.0
5	100.0	124879.0
6	100.0	124879.0
7	100.0	124879.0
8	100.0	124879.0
9	100.0	124879.0
10	100.0	124879.0

Fit of model to data used for modeling ?

3DEM volume

Validation for this section is under development.

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 lab](#) contributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.