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	8ZZ1
PDB-Dev ID	PDBDEV_00000001
Structure Title	Structure of the Nup84 sub-complex of the Nuclear Pore Complex
Structure Authors	Shi Y; Fernandez-Martinez J; Tjioe E; Pellarin R; Kim SJ; Williams R; Schneidman-Duhovny D; Sali A; Rout MP; Chait BT

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

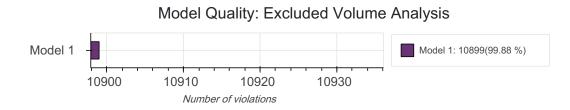
We welcome your comments at pdb-dev@mail.wwpdb.org

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.

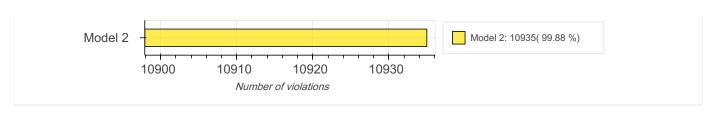
Overall quality o

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 2 distinct ensemble(s).

Summary ?

This entry consists of 2 unique models, with 7 subunits in each model. A total of 28 datasets or restraints were used to build this entry. Each model is represented by 40 rigid bodies and 42 flexible or non-rigid units.

Entry composition?

There are 2 unique types of models in this entry. These models are titled Cluster 1/Best scoring model, Cluster 2/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Nup84	А	А	726
1	2	2	Nup85	В	В	744
1	3	3	Nup120	С	С	1037
1	4	4	Nup133	D	D	1157
1	5	5	Nup145c	E	E	712
1	6	6	Seh1	F	F	349
1	7	7	Sec13	G	G	297
2	1	1	Nup84	А	А	726
2	2	2	Nup85	В	В	744
2	3	3	Nup120	С	С	1037
2	4	4	Nup133	D	D	1157

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
2	5	5	Nup145c	E	E	712
2	6	6	Seh1	F	F	349
2	7	7	Sec13	G	G	297

Datasets used for modeling

There are 28 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	3JRO
2	Experimental model	PDB	3F3F
3	Experimental model	PDB	ЗІКО
4	Comparative model	File	10.5281/zenodo.1218053
5	Experimental model	PDB	3CQC
6	Comparative model	File	10.5281/zenodo.1218053
7	Experimental model	PDB	4LCT
8	Experimental model	PDB	2QX5
9	Experimental model	PDB	3EWE
10	Comparative model	File	10.5281/zenodo.1218053
11	Experimental model	PDB	3F7F
12	Experimental model	PDB	3HXR
13	Experimental model	PDB	4FHN
14	Comparative model	File	10.5281/zenodo.1218053
15	Experimental model	PDB	4Q9T
16	Comparative model	File	10.5281/zenodo.1218053

ID	Dataset type	Database name	Data access code
17	Experimental model	PDB	314R
18	Experimental model	PDB	3KFO
19	Comparative model	File	10.5281/zenodo.1218053
20	Experimental model	PDB	3BG1
21	Experimental model	PDB	3BG0
22	Comparative model	File	10.5281/zenodo.1218053
23	Experimental model	PDB	3F3F
24	Experimental model	PDB	2PM7
25	Crosslinking-MS data	File	10.5281/zenodo.1218053
26	Crosslinking-MS data	File	10.5281/zenodo.1218053
27	EM raw micrographs	File	10.5281/zenodo.58025
28	2DEM class average	File	10.5281/zenodo.1218053

Representation ?

This entry has only one representation and includes 40 rigid bodies and 42 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
в	67-122, 135-427, 461-529, 533-602, 620-671, 680- 743	1-66, 123-134, 428-460, 530-532, 603-619, 672-679, 744-744
С	1-29, 53-212, 221-305, 311-429, 440-710, 711-712, 727-781, 805-892, 903-910, 921-1010, 1023-1037	30-52, 213-220, 306-310, 430-439, 713-726, 782-804, 893-902, 911-920, 1011-1022
D	56-78, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 79-85, 126-132, 145-161, 185-192, 201- 205, 250-257, 481-489, 764-771, 1156-1157

Chain ID	Rigid bodies	Non-rigid segments
E	126-144, 151-175, 182-553	1-125, 145-150, 176-181, 554-712
F	1-248, 288-346	249-287, 347-349
G	2-158, 166-296	1-1, 159-165, 297-297

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	Replica exchange monte carlo	Sampling	None	500	False	True
2	1	Replica exchange monte carlo	Sampling	None	5000	False	True

There are 6 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	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/hhpred
4	PSIPRED	4.0	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
5	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/? disopred=1

ID	Software name	Software version	Software classification	Software location
6	MODELLER	9.12	comparative modeling	https://salilab.org/modeller/

Data quality

Crosslinking-MS

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

EM raw micrographs

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity 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	99.88	10899.0
2	99.88	10935.0

Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

2DEM class average

Validation for this section is under development.

EM raw micrographs

Validation for this section is under development.

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Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

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