Integrative Structure Validation Report

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

Integrative Modeling Validation Version 1.0
Integrative Modeling Platform Version 2.15.0

PDB ID	PDBDEV_00000001
Structure Name	Structure of the Nup84 sub-complex of the Nuclear Pore Complex
Publication Title	Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptameric module from the nuclear pore complex.
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.

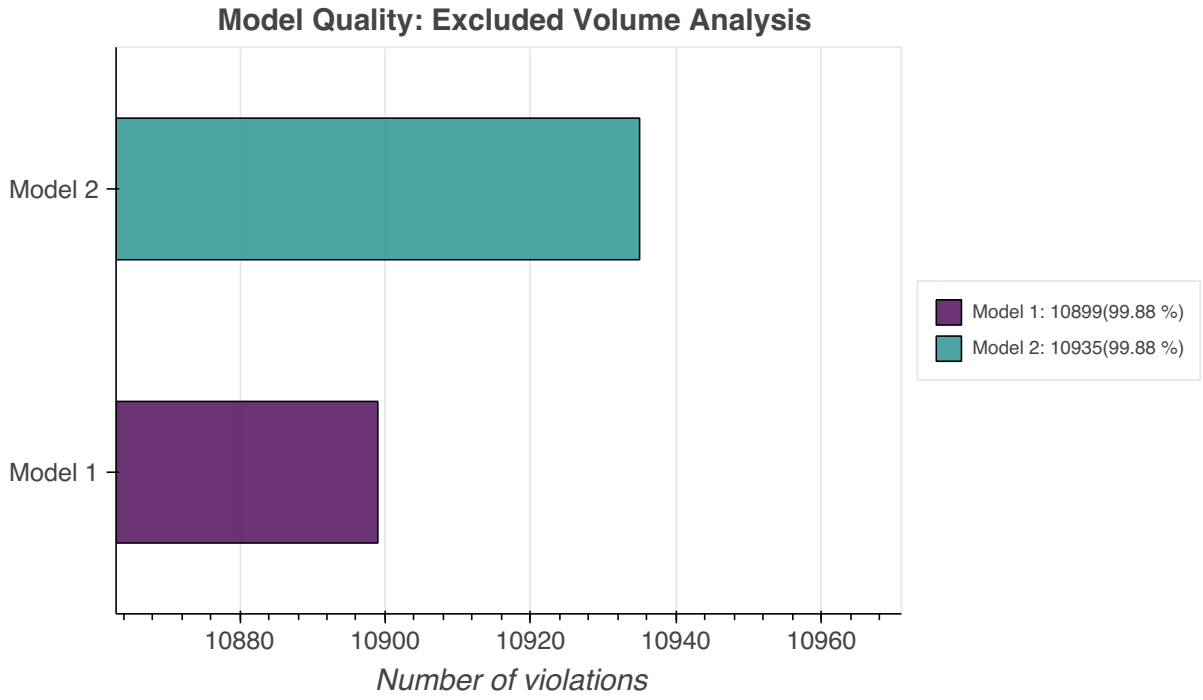
We welcome your comments at pdb-dev@mail.wwpdb.org

A user guide is available at https://pdb-dev-beta.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.



Ensemble information

This entry consists of 2 distinct ensembles.

Summary

This entry consists of 2 unique models, with 7 subunits in each model. A total of 28 datasets or restraints was 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	Total residues
1	1	1	Nup84	A	726
1	2	2	Nup85	B	744
1	3	3	Nup120	C	1037

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	4	4	Nup133	D	1157
1	5	5	Nup145c	E	712
1	6	6	Seh1	F	349
1	7	7	Sec13	G	297
2	1	1	Nup84	A	726
2	2	2	Nup85	B	744
2	3	3	Nup120	C	1037
2	4	4	Nup133	D	1157
2	5	5	Nup145c	E	712
2	6	6	Seh1	F	349
2	7	7	Sec13	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	3IKO
4	Comparative model	Not available	None
5	Experimental model	PDB	3CQC
6	Comparative model	Not available	None
7	Experimental model	PDB	4LCT
8	Experimental model	PDB	2QX5

ID	Dataset type	Database name	Data access code
9	Experimental model	PDB	3EWE
10	Comparative model	Not available	None
11	Experimental model	PDB	3F7F
12	Experimental model	PDB	3HXR
13	Experimental model	PDB	4FHN
14	Comparative model	Not available	None
15	Experimental model	PDB	4Q9T
16	Comparative model	Not available	None
17	Experimental model	PDB	3I4R
18	Experimental model	PDB	3KFO
19	Comparative model	Not available	None
20	Experimental model	PDB	3BG1
21	Experimental model	PDB	3BG0
22	Comparative model	Not available	None
23	Experimental model	PDB	3F3F
24	Experimental model	PDB	2PM7
25	CX-MS data	Not available	None
26	CX-MS data	Not available	None
27	EM raw micrographs	Not available	None
28	2DEM class average	Not available	None

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:Comparative model/None, 27-80:Comparative model/None, 96-126:Comparative model/None, 136-364:Comparative model/None, 372-483:Comparative model/None, 506-562:Comparative model/None, 575-726:Comparative model/None.	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574.
B	67-122:Comparative model/None, 135-427:Comparative model/None, 461-529:Comparative model/None, 533-602:Comparative model/None, 620-671:Comparative model/None, 680-743:Comparative model/None.	1-66, 123-134, 428-460, 530-532, 603-619, 672-679, 744-744.
C	1-29:Comparative model/None, 53-212:Comparative model/None, 221-305:Comparative model/None, 311-429:Comparative model/None, 440-710:Comparative model/None, 711-712:Comparative model/None, 727-781:Comparative model/None, 805-892:Comparative model/None, 903-910:Comparative model/None, 921-1010:Comparative model/None, 1023-1037:Comparative model/None.	30-52, 213-220, 306-310, 430-439, 713-726, 782-804, 893-902, 911-920, 1011-1022.
D	56-78:Comparative model/None, 86-125:Comparative model/None, 133-144:Comparative model/None, 162-184:Comparative model/None, 193-200:Comparative model/None, 206-249:Comparative model/None, 258-480:Comparative model/None, 490-763:Comparative model/None, 772-1155:Comparative model/None.	1-55, 79-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157.
E	126-144:Comparative model/None, 151-175:Comparative model/None, 182-553:Comparative model/None.	1-125, 145-150, 176-181, 554-712.
F	1-248:Experimental model/3F3F, 288-346:Experimental model/3F3F.	249-287, 347-349.
G	2-158:Experimental model/2PM7, 166-296:Experimental model/2PM7.	1-1, 159-165, 297-297.

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	500	False	True

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
2	1	Replica exchange monte carlo	Sampling	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
6	MODELLER	9.12	comparative modeling	https://salilab.org/modeller/

Data quality

CX-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

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

CX-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.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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