Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

PDB ID	PDBDEV00000010
Molecule Name	Integrative structure and functional anatomy of a single spoke of a nuclear pore complex
Title	Integrative structure and functional anatomy of a nuclear pore complex.
Authors	Kim SJ;Fernandez-Martinez J;Nudelman I;Shi Y;Zhang W;Raveh B;Herricks T;Slaughter BD;Hogan JA;Upla P;Chemmama IE;Pellarin R;Echeverria I;Shivaraju M;Chaudhury AS;Wang J;Williams R;Unruh JR;Greenberg CH;Jacobs EY;Yu Z;de la Cruz MJ;Mironska R;Stokes DL;Aitchison JD;Jarrold MF;Gerton JL;Ludtke SJ;Akey CW;Chait BT;Sali A;Rout MP

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

Integrative Modeling Package : Version XX
Molprobity : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There are 36 unique types of models in this entry. Models have
69,54,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Nup84	A	726
1	Nup85	H	726
1	Nup120	B	744
1	Nup133	I	744
1	Nup145c	C	1037
1	Seh1	J	1037
1	Sec13	D	1157
1	Dyn2	K	1157
1	Nup82	E	712
1	Nup159	L	712

1	Nup133	L	712
1	Nsp1	F	349
1	Nic96	M	349
1	Nup49	G	297
1	Nup57	N	297
1	Nup157	O	92
1	Nup170	P	92
1	Nup188	Q	713
1	Nup192	R	713
1	Nup53	S	1460
1	Nup59	T	1460
1	Ndc1	U	823
1	Pom34	V	823
1	Pom152	X	823
1	Nup100	AB	823
1	Nup116	AF	823
1	Nup42	AJ	823
1	Gle1	W	839
1	Nup145	AA	839
1	Nup1	AE	839
1	Nup60	AI	839
1	Mlp1	Y	472
1	Mlp2	AC	472
1	Nup84	AG	472
1	Nup85	AK	472
1	Nup120	Z	541
1	Nup133	AD	541
1	Nup145c	AH	541
1	Seh1	AL	541
1	Sec13	AM	1391
1	Dyn2	AQ	1391

1	Nup82	AN	1502
1	Nup159	AR	1502
1	Nsp1	AO	1655
1	Nic96	AS	1655
1	Nup49	AP	1683
1	Nup57	AT	1683
1	Nup157	AU	475
1	Nup170	AZ	475
1	Nup188	AV	528
1	Nup192	BA	528
1	Nup53	AW	655
1	Nup59	BB	655
1	Ndc1	AX	299
1	Pom34	BC	299
1	Pom152	AY	1337
1	Nup100	BD	1337
1	Nup116	BE	959
1	Nup42	BF	959
1	Gle1	BG	1113
1	Nup145	BH	1113
1	Nup1	BI	430
1	Nup60	BJ	538
1	Mlp1	BK	1317
1	Mlp2	BL	1317
1	Nup84	BM	1076
1	Nup85	BN	539
1	Nup120	BO	539
1	Nup133	BP	1875
1	Nup145c	BQ	1679

There are 13 software packages reported in this entry.

iD	Software Name		Software Version	Software Classification

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	HHpred	2.0.16	protein homology detection
4	PSIPRED	4.0	secondary structure prediction
5	DISOPRED	3	disorder prediction
6	DomPred	None	domain boundary prediction
7	COILS/PCOILS	None	coiled-coil prediction
8	EMAN2	2.2	image processing
9	RELION	1.4	image processing
10	SGD	None	database
11	HeliQuest	None	helix prediction
12	MODELLER	9.15	comparative modeling
13	MODELLER	9.13	comparative modeling

There are 65 unique datasets used to build the model in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	Integrative model	Not Listed	None
2	Integrative model	Not Listed	None
3	Experimental model	PDB	5CWS
4	Comparative model	Not Listed	None
5	Experimental model	PDB	2QX5
6	Experimental model	Not Listed	None
7	Experimental model	Not Listed	None
8	Comparative model	Not Listed	None
9	Comparative model	Not Listed	None
10	Comparative model	Not Listed	None
11	Comparative model	Not Listed	None
12	Comparative model	Not Listed	None
13	Comparative model	Not Listed	None
14	Integrative model	Not Listed	None

15	Integrative model	Not Listed	None
16	Experimental model	PDB	3NF5
17	Comparative model	Not Listed	None
18	Comparative model	Not Listed	None
19	Experimental model	PDB	3KEP
20	Experimental model	Not Listed	None
21	Mass Spectrometry data	Not Listed	None
22	CX-MS data	Not Listed	None
23	CX-MS data	Not Listed	None
24	EM raw micrographs	EMPIAR	EMPIAR-10155
25	3DEM volume	EMDB	EMD-7321
26	3DEM volume	Not Listed	None
27	SAS data	Not Listed	None
28	SAS data	Not Listed	None
29	SAS data	Not Listed	None
30	SAS data	Not Listed	None
31	SAS data	Not Listed	None
32	SAS data	Not Listed	None
33	SAS data	Not Listed	None
34	SAS data	Not Listed	None
35	SAS data	Not Listed	None
36	SAS data	Not Listed	None
37	SAS data	Not Listed	None
38	SAS data	Not Listed	None
39	SAS data	Not Listed	None
40	SAS data	Not Listed	None
41	SAS data	Not Listed	None
42	SAS data	Not Listed	None
43	SAS data	Not Listed	None
44	SAS data	Not Listed	None

45	SAS data	Not Listed	None
46	SAS data	Not Listed	None
47	SAS data	Not Listed	None
48	SAS data	SASBDB	SASDBV9
49	SAS data	SASBDB	SASDBW9
50	SAS data	SASBDB	SASDBZ9
51	SAS data	SASBDB	SASDBX9
52	SAS data	SASBDB	SASDBY9
53	SAS data	Not Listed	None
54	SAS data	Not Listed	None
55	SAS data	Not Listed	None
56	SAS data	Not Listed	None
57	SAS data	Not Listed	None
58	SAS data	Not Listed	None
59	SAS data	Not Listed	None
60	SAS data	Not Listed	None
61	SAS data	Not Listed	None
62	SAS data	Not Listed	None
63	EM raw micrographs	EMPIAR	EMPIAR-10162
64	2DEM class average	Not Listed	None
65	2DEM class average	Not Listed	None

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertaintiy of model