

# Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

PDB ID	PDBDEV00000012
Molecule Name	Integrative structure and functional anatomy of eight spokes 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;Chemmam 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*  
*Molprobit : Version XX*  
*Phenix : Version XX*  
*Integrative Modeling Validation Package : Version XX*

## 1. Overall quality at a glance

## 2. Entry composition

There are 37 unique types of models in this entry. Models have 552,200,54,1 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Nup84	A	726
1	Nup85	H	726
1	Nup120	BR	726
1	Nup133	BY	726
1	Nup145c	CF	726
1	Seh1	CM	726
1	Sec13	CT	726
1	Dyn2	DA	726
1	Nup82	DH	726
1	Nup159	DO	726

	Nup133	DC	726
1	Nsp1	DV	726
1	Nic96	EC	726
1	Nup49	EJ	726
1	Nup57	EQ	726
1	Nup157	EX	726
1	Nup170	FE	726
1	Nup188	B	744
1	Nup192	I	744
1	Nup53	BS	744
1	Nup59	BZ	744
1	Ndc1	CG	744
1	Pom34	CN	744
1	Pom152	CU	744
1	Nup100	DB	744
1	Nup116	DI	744
1	Nup42	DP	744
1	Gle1	DW	744
1	Nup145	ED	744
1	Nup1	EK	744
1	Nup60	ER	744
1	Mlp1	EY	744
1	Mlp2	FF	744
1	Nup84	C	1037
1	Nup85	J	1037
1	Nup120	BT	1037
1	Nup133	CA	1037
1	Nup145c	CH	1037
1	Seh1	CO	1037
1	Sec13	CV	1037
1	Dyn2	DC	1037

1	Nup82	DJ	1037
1	Nup159	DQ	1037
1	Nsp1	DX	1037
1	Nic96	EE	1037
1	Nup49	EL	1037
1	Nup57	ES	1037
1	Nup157	EZ	1037
1	Nup170	FG	1037
1	Nup188	D	1157
1	Nup192	K	1157
1	Nup53	BU	1157
1	Nup59	CB	1157
1	Ndc1	CI	1157
1	Pom34	CP	1157
1	Pom152	CW	1157
1	Nup100	DD	1157
1	Nup116	DK	1157
1	Nup42	DR	1157
1	Gle1	DY	1157
1	Nup145	EF	1157
1	Nup1	EM	1157
1	Nup60	ET	1157
1	Mlp1	FA	1157
1	Mlp2	FH	1157
1	Nup84	E	712
1	Nup85	L	712
1	Nup120	BV	712
1	Nup133	CC	712
1	Nup145c	CJ	712
1	Seh1	CQ	712
1	Sec13	CX	712

1	Dyn2	DE	712
1	Nup82	DL	712
1	Nup159	DS	712
1	Nsp1	DZ	712
1	Nic96	EG	712
1	Nup49	EN	712
1	Nup57	EU	712
1	Nup157	FB	712
1	Nup170	FI	712
1	Nup188	F	349
1	Nup192	M	349
1	Nup53	BW	349
1	Nup59	CD	349
1	Ndc1	CK	349
1	Pom34	CR	349
1	Pom152	CY	349
1	Nup100	DF	349
1	Nup116	DM	349
1	Nup42	DT	349
1	Gle1	EA	349
1	Nup145	EH	349
1	Nup1	EO	349
1	Nup60	EV	349
1	Mlp1	FC	349
1	Mlp2	FJ	349
1	Nup84	G	297
1	Nup85	N	297
1	Nup120	BX	297
1	Nup133	CE	297
1	Nup145c	CL	297
1	Seh1	CS	297

1	Sec13	CZ	297
1	Dyn2	DG	297
1	Nup82	DN	297
1	Nup159	DU	297
1	Nsp1	EB	297
1	Nic96	EI	297
1	Nup49	EP	297
1	Nup57	EW	297
1	Nup157	FD	297
1	Nup170	FK	297
1	Nup188	O	92
1	Nup192	P	92
1	Nup53	FL	92
1	Nup59	FM	92
1	Ndc1	FT	92
1	Pom34	FU	92
1	Pom152	GB	92
1	Nup100	GC	92
1	Nup116	GJ	92
1	Nup42	GK	92
1	Gle1	GR	92
1	Nup145	GS	92
1	Nup1	GZ	92
1	Nup60	HA	92
1	Mlp1	HH	92
1	Mlp2	HI	92
1	Nup84	Q	713
1	Nup85	R	713
1	Nup120	FN	713
1	Nup133	FO	713
1	Nup145c	FV	713

1	Seh1	FW	713
1	Sec13	GD	713
1	Dyn2	GE	713
1	Nup82	GL	713
1	Nup159	GM	713
1	Nsp1	GT	713
1	Nic96	GU	713
1	Nup49	HB	713
1	Nup57	HC	713
1	Nup157	HJ	713
1	Nup170	HK	713
1	Nup188	S	1460
1	Nup192	T	1460
1	Nup53	FP	1460
1	Nup59	FQ	1460
1	Ndc1	FX	1460
1	Pom34	FY	1460
1	Pom152	GF	1460
1	Nup100	GG	1460
1	Nup116	GN	1460
1	Nup42	GO	1460
1	Gle1	GV	1460
1	Nup145	GW	1460
1	Nup1	HD	1460
1	Nup60	HE	1460
1	Mlp1	HL	1460
1	Mlp2	HM	1460
1	Nup84	U	823
1	Nup85	V	823
1	Nup120	X	823
1	Nup133	AR	823

	Nup100	AF	823
1	Nup145c	AF	823
1	Seh1	AJ	823
1	Sec13	FR	823
1	Dyn2	FS	823
1	Nup82	FZ	823
1	Nup159	GA	823
1	Nsp1	GH	823
1	Nic96	GI	823
1	Nup49	GP	823
1	Nup57	GQ	823
1	Nup157	GX	823
1	Nup170	GY	823
1	Nup188	HF	823
1	Nup192	HG	823
1	Nup53	HN	823
1	Nup59	HO	823
1	Ndc1	HR	823
1	Pom34	HS	823
1	Pom152	HZ	823
1	Nup100	IA	823
1	Nup116	IH	823
1	Nup42	II	823
1	Gle1	IP	823
1	Nup145	IQ	823
1	Nup1	IX	823
1	Nup60	IY	823
1	Mlp1	JF	823
1	Mlp2	JG	823
1	Nup84	JN	823
1	Nup85	JO	823

1	Nup120	JV	823
1	Nup133	JW	823
1	Nup145c	KD	823
1	Seh1	KE	823
1	Sec13	KL	823
1	Dyn2	KM	823
1	Nup82	KT	823
1	Nup159	KU	823
1	Nsp1	LB	823
1	Nic96	LC	823
1	Nup49	LJ	823
1	Nup57	LK	823
1	Nup157	LR	823
1	Nup170	LS	823
1	Nup188	W	839
1	Nup192	AA	839
1	Nup53	AE	839
1	Nup59	AI	839
1	Ndc1	HP	839
1	Pom34	HQ	839
1	Pom152	HX	839
1	Nup100	HY	839
1	Nup116	IF	839
1	Nup42	IG	839
1	Gle1	IN	839
1	Nup145	IO	839
1	Nup1	IV	839
1	Nup60	IW	839
1	Mlp1	JD	839
1	Mlp2	JE	839
1	Nup84	JL	839



1	Nup85	JM	839
1	Nup120	JT	839
1	Nup133	JU	839
1	Nup145c	KB	839
1	Seh1	KC	839
1	Sec13	KJ	839
1	Dyn2	KK	839
1	Nup82	KR	839
1	Nup159	KS	839
1	Nsp1	KZ	839
1	Nic96	LA	839
1	Nup49	LH	839
1	Nup57	LI	839
1	Nup157	LP	839
1	Nup170	LQ	839
1	Nup188	Y	472
1	Nup192	AC	472
1	Nup53	AG	472
1	Nup59	AK	472
1	Ndc1	HT	472
1	Pom34	HU	472
1	Pom152	IB	472
1	Nup100	IC	472
1	Nup116	IJ	472
1	Nup42	IK	472
1	Gle1	IR	472
1	Nup145	IS	472
1	Nup1	IZ	472
1	Nup60	JA	472
1	Mlp1	JH	472
1	Mlp2	JI	472

1	Nup84	JP	472
1	Nup85	JQ	472
1	Nup120	JX	472
1	Nup133	JY	472
1	Nup145c	KF	472
1	Seh1	KG	472
1	Sec13	KN	472
1	Dyn2	KO	472
1	Nup82	KV	472
1	Nup159	KW	472
1	Nsp1	LD	472
1	Nic96	LE	472
1	Nup49	LL	472
1	Nup57	LM	472
1	Nup157	LT	472
1	Nup170	LU	472
1	Nup188	Z	541
1	Nup192	AD	541
1	Nup53	AH	541
1	Nup59	AL	541
1	Ndc1	HV	541
1	Pom34	HW	541
1	Pom152	ID	541
1	Nup100	IE	541
1	Nup116	IL	541
1	Nup42	IM	541
1	Gle1	IT	541
1	Nup145	IU	541
1	Nup1	JB	541
1	Nup60	JC	541
1	Mlp1	JJ	541

1	Mlp2	JK	541
1	Nup84	JR	541
1	Nup85	JS	541
1	Nup120	JZ	541
1	Nup133	KA	541
1	Nup145c	KH	541
1	Seh1	KI	541
1	Sec13	KP	541
1	Dyn2	KQ	541
1	Nup82	KX	541
1	Nup159	KY	541
1	Nsp1	LF	541
1	Nic96	LG	541
1	Nup49	LN	541
1	Nup57	LO	541
1	Nup157	LV	541
1	Nup170	LW	541
1	Nup188	AM	1391
1	Nup192	AQ	1391
1	Nup53	LX	1391
1	Nup59	MB	1391
1	Ndc1	MF	1391
1	Pom34	MJ	1391
1	Pom152	MN	1391
1	Nup100	MR	1391
1	Nup116	MV	1391
1	Nup42	MZ	1391
1	Gle1	ND	1391
1	Nup145	NH	1391
1	Nup1	NL	1391
1	Nup60	NP	1391

	Protein	Category	Accession
1	Mlp1	NT	1391
1	Mlp2	NX	1391
1	Nup84	AN	1502
1	Nup85	AR	1502
1	Nup120	LY	1502
1	Nup133	MC	1502
1	Nup145c	MG	1502
1	Seh1	MK	1502
1	Sec13	MO	1502
1	Dyn2	MS	1502
1	Nup82	MW	1502
1	Nup159	NA	1502
1	Nsp1	NE	1502
1	Nic96	NI	1502
1	Nup49	NM	1502
1	Nup57	NQ	1502
1	Nup157	NU	1502
1	Nup170	NY	1502
1	Nup188	AO	1655
1	Nup192	AS	1655
1	Nup53	LZ	1655
1	Nup59	MD	1655
1	Ndc1	MH	1655
1	Pom34	ML	1655
1	Pom152	MP	1655
1	Nup100	MT	1655
1	Nup116	MX	1655
1	Nup42	NB	1655
1	Gle1	NF	1655
1	Nup145	NJ	1655
1	Nup133	NC	1655

1	Nup1	NN	1655
1	Nup60	NR	1655
1	Mlp1	NV	1655
1	Mlp2	NZ	1655
1	Nup84	AP	1683
1	Nup85	AT	1683
1	Nup120	MA	1683
1	Nup133	ME	1683
1	Nup145c	MI	1683
1	Seh1	MM	1683
1	Sec13	MQ	1683
1	Dyn2	MU	1683
1	Nup82	MY	1683
1	Nup159	NC	1683
1	Nsp1	NG	1683
1	Nic96	NK	1683
1	Nup49	NO	1683
1	Nup57	NS	1683
1	Nup157	NW	1683
1	Nup170	OA	1683
1	Nup188	AU	475
1	Nup192	AZ	475
1	Nup53	OB	475
1	Nup59	OG	475
1	Ndc1	OL	475
1	Pom34	OQ	475
1	Pom152	OV	475
1	Nup100	PA	475
1	Nup116	PF	475
1	Nup42	PK	475
1	Gle1	PP	475

1	Nup145	PU	475
1	Nup1	PZ	475
1	Nup60	QE	475
1	Mlp1	QJ	475
1	Mlp2	QO	475
1	Nup84	AV	528
1	Nup85	BA	528
1	Nup120	OC	528
1	Nup133	OH	528
1	Nup145c	OM	528
1	Seh1	OR	528
1	Sec13	OW	528
1	Dyn2	PB	528
1	Nup82	PG	528
1	Nup159	PL	528
1	Nsp1	PQ	528
1	Nic96	PV	528
1	Nup49	QA	528
1	Nup57	QF	528
1	Nup157	QK	528
1	Nup170	QP	528
1	Nup188	AW	655
1	Nup192	BB	655
1	Nup53	OD	655
1	Nup59	OI	655
1	Ndc1	ON	655
1	Pom34	OS	655
1	Pom152	OX	655
1	Nup100	PC	655
1	Nup116	PH	655
1	Nup42	PM	655

1	Gle1	PR	655
1	Nup145	PW	655
1	Nup1	QB	655
1	Nup60	QG	655
1	Mlp1	QL	655
1	Mlp2	QQ	655
1	Nup84	AX	299
1	Nup85	BC	299
1	Nup120	OE	299
1	Nup133	OJ	299
1	Nup145c	OO	299
1	Seh1	OT	299
1	Sec13	OY	299
1	Dyn2	PD	299
1	Nup82	PI	299
1	Nup159	PN	299
1	Nsp1	PS	299
1	Nic96	PX	299
1	Nup49	QC	299
1	Nup57	QH	299
1	Nup157	QM	299
1	Nup170	QR	299
1	Nup188	AY	1337
1	Nup192	BD	1337
1	Nup53	OF	1337
1	Nup59	OK	1337
1	Ndc1	OP	1337
1	Pom34	OU	1337
1	Pom152	OZ	1337
1	Nup100	PE	1337
1	Nup116	PJ	1337

1	Nup42	PO	1337
1	Gle1	PT	1337
1	Nup145	PY	1337
1	Nup1	QD	1337
1	Nup60	QI	1337
1	Mlp1	QN	1337
1	Mlp2	QS	1337
1	Nup84	BE	959
1	Nup85	BF	959
1	Nup120	QT	959
1	Nup133	QU	959
1	Nup145c	QZ	959
1	Seh1	RA	959
1	Sec13	RF	959
1	Dyn2	RG	959
1	Nup82	RL	959
1	Nup159	RM	959
1	Nsp1	RR	959
1	Nic96	RS	959
1	Nup49	RX	959
1	Nup57	RY	959
1	Nup157	SD	959
1	Nup170	SE	959
1	Nup188	BG	1113
1	Nup192	BH	1113
1	Nup53	QV	1113
1	Nup59	QW	1113
1	Ndc1	RB	1113
1	Pom34	RC	1113
1	Pom152	RH	1113
1	Nup100	RI	1113



1	Nup116	RN	1113
1	Nup42	RO	1113
1	Gle1	RT	1113
1	Nup145	RU	1113
1	Nup1	RZ	1113
1	Nup60	SA	1113
1	Mlp1	SF	1113
1	Mlp2	SG	1113
1	Nup84	BI	430
1	Nup85	QX	430
1	Nup120	RD	430
1	Nup133	RJ	430
1	Nup145c	RP	430
1	Seh1	RV	430
1	Sec13	SB	430
1	Dyn2	SH	430
1	Nup82	BJ	538
1	Nup159	QY	538
1	Nsp1	RE	538
1	Nic96	RK	538
1	Nup49	RQ	538
1	Nup57	RW	538
1	Nup157	SC	538
1	Nup170	SI	538
1	Nup188	BK	1317
1	Nup192	BL	1317
1	Nup53	SJ	1317
1	Nup59	SK	1317
1	Ndc1	SO	1317
1	Pom34	SP	1317
1	Pom159	ST	1317

1	Pom152	ST	1317
1	Nup100	SU	1317
1	Nup116	SY	1317
1	Nup42	SZ	1317
1	Gle1	TD	1317
1	Nup145	TE	1317
1	Nup1	TI	1317
1	Nup60	TJ	1317
1	Mlp1	TN	1317
1	Mlp2	TO	1317
1	Nup84	BM	1076
1	Nup85	SN	1076
1	Nup120	SS	1076
1	Nup133	SX	1076
1	Nup145c	TC	1076
1	Seh1	TH	1076
1	Sec13	TM	1076
1	Dyn2	TR	1076
1	Nup82	BN	539
1	Nup159	BO	539
1	Nsp1	SL	539
1	Nic96	SM	539
1	Nup49	SQ	539
1	Nup57	SR	539
1	Nup157	SV	539
1	Nup170	SW	539
1	Nup188	TA	539
1	Nup192	TB	539
1	Nup53	TF	539
1	Nup59	TG	539
1	Ndc1	TK	539

1	Pom34	TL	539
1	Pom152	TP	539
1	Nup100	TQ	539
1	Nup116	BP	1875
1	Nup42	TS	1875
1	Gle1	TU	1875
1	Nup145	TW	1875
1	Nup1	TY	1875
1	Nup60	UA	1875
1	Mlp1	UC	1875
1	Mlp2	UE	1875
1	Nup84	BQ	1679
1	Nup85	TT	1679
1	Nup120	TV	1679
1	Nup133	TX	1679
1	Nup145c	TZ	1679
1	Seh1	UB	1679
1	Sec13	UD	1679
1	Dyn2	UF	1679

There are 13 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	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

ET	EM raw micrographs	EM data	EM data PDB
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

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### 3. Data quality

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### 4. Model quality

#### 4.1 Too-close contacts

#### 4.2 Torsion angles

##### 4.2.1 Protein backbone

##### 4.2.2 Protein sidechains

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### 5. Fit of model and data

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### 6. Uncertainty of model

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