

# Full wwPDB Integrative Structure Validation Report

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PDB ID	PDBDEV00000011
Molecule Name	Integrative structure and functional anatomy of three 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 1 unique types of models in this entry. The entry contains 295 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Nup84	A	726
1	Nup85	H	726
1	Nup120	O	726
1	Nup133	V	726
1	Nup145c	AC	726
1	Seh1	AJ	726
1	Sec13	B	744
1	Dyn2	I	744
1	Nup82	P	744
1	Nup159	W	744

1	Nsp1	AD	744
1	Nic96	AK	744
1	Nup49	C	1037
1	Nup57	J	1037
1	Nup157	Q	1037
1	Nup170	X	1037
1	Nup188	AE	1037
1	Nup192	AL	1037
1	Nup53	D	1157
1	Nup59	K	1157
1	Ndc1	R	1157
1	Pom34	Y	1157
1	Pom152	AF	1157
1	Nup100	AM	1157
1	Nup116	E	712
1	Nup42	L	712
1	Gle1	S	712
1	Nup145	Z	712
1	Nup1	AG	712
1	Nup60	AN	712
1	Mlp1	F	349
1	Mlp2	M	349
1	Nup84	T	349
1	Nup85	AA	349
1	Nup120	AH	349
1	Nup133	AO	349
1	Nup145c	G	297
1	Seh1	N	297
1	Sec13	U	297
1	Dyn2	AB	297
1	Nup82	AI	297

1	Nup159	AP	297
1	Nsp1	AQ	92
1	Nic96	AR	92
1	Nup49	AY	92
1	Nup57	AZ	92
1	Nup157	BG	92
1	Nup170	BH	92
1	Nup188	AS	713
1	Nup192	AT	713
1	Nup53	BA	713
1	Nup59	BB	713
1	Ndc1	BI	713
1	Pom34	BJ	713
1	Pom152	AU	1460
1	Nup100	AV	1460
1	Nup116	BC	1460
1	Nup42	BD	1460
1	Gle1	BK	1460
1	Nup145	BL	1460
1	Nup1	AW	823
1	Nup60	AX	823
1	Mlp1	BE	823
1	Mlp2	BF	823
1	Nup84	BM	823
1	Nup85	BN	823
1	Nup120	BP	823
1	Nup133	BT	823
1	Nup145c	BX	823
1	Seh1	CB	823
1	Sec13	CF	823
1	Dvn2	C.I	823

	Gene	CC	SEC
1	Nup82	CN	823
1	Nup159	CR	823
1	Nsp1	CV	823
1	Nic96	CZ	823
1	Nup49	DD	823
1	Nup57	DH	823
1	Nup157	BO	839
1	Nup170	BS	839
1	Nup188	BW	839
1	Nup192	CA	839
1	Nup53	CE	839
1	Nup59	CI	839
1	Ndc1	CM	839
1	Pom34	CQ	839
1	Pom152	CU	839
1	Nup100	CY	839
1	Nup116	DC	839
1	Nup42	DG	839
1	Gle1	BQ	472
1	Nup145	BU	472
1	Nup1	BY	472
1	Nup60	CC	472
1	Mlp1	CG	472
1	Mlp2	CK	472
1	Nup84	CO	472
1	Nup85	CS	472
1	Nup120	CW	472
1	Nup133	DA	472
1	Nup145c	DE	472
1	Seh1	DI	472

1	Sec13	BR	541
1	Dyn2	BV	541
1	Nup82	BZ	541
1	Nup159	CD	541
1	Nsp1	CH	541
1	Nic96	CL	541
1	Nup49	CP	541
1	Nup57	CT	541
1	Nup157	CX	541
1	Nup170	DB	541
1	Nup188	DF	541
1	Nup192	DJ	541
1	Nup53	DK	1391
1	Nup59	DO	1391
1	Ndc1	DS	1391
1	Pom34	DW	1391
1	Pom152	EA	1391
1	Nup100	EE	1391
1	Nup116	DL	1502
1	Nup42	DP	1502
1	Gle1	DT	1502
1	Nup145	DX	1502
1	Nup1	EB	1502
1	Nup60	EF	1502
1	Mlp1	DM	1655
1	Mlp2	DQ	1655
1	Nup84	DU	1655
1	Nup85	DY	1655
1	Nup120	EC	1655
1	Nup133	EG	1655
1	Nup145c	DN	1683

1	Seh1	DR	1683
1	Sec13	DV	1683
1	Dyn2	DZ	1683
1	Nup82	ED	1683
1	Nup159	EH	1683
1	Nsp1	EI	475
1	Nic96	EN	475
1	Nup49	ES	475
1	Nup57	EX	475
1	Nup157	FC	475
1	Nup170	FH	475
1	Nup188	EJ	528
1	Nup192	EO	528
1	Nup53	ET	528
1	Nup59	EY	528
1	Ndc1	FD	528
1	Pom34	FI	528
1	Pom152	EK	655
1	Nup100	EP	655
1	Nup116	EU	655
1	Nup42	EZ	655
1	Gle1	FE	655
1	Nup145	FJ	655
1	Nup1	EL	299
1	Nup60	EQ	299
1	Mlp1	EV	299
1	Mlp2	FA	299
1	Nup84	FF	299
1	Nup85	FK	299
1	Nup120	EM	1337
1	Nup133	ER	1337

1	Nup145c	EW	1337
1	Seh1	FB	1337
1	Sec13	FG	1337
1	Dyn2	FL	1337
1	Nup82	FM	959
1	Nup159	FN	959
1	Nsp1	FS	959
1	Nic96	FT	959
1	Nup49	FY	959
1	Nup57	FZ	959
1	Nup157	FO	1113
1	Nup170	FP	1113
1	Nup188	FU	1113
1	Nup192	FV	1113
1	Nup53	GA	1113
1	Nup59	GB	1113
1	Ndc1	FQ	430
1	Pom34	FW	430
1	Pom152	GC	430
1	Nup100	FR	538
1	Nup116	FX	538
1	Nup42	GD	538
1	Gle1	GE	1317
1	Nup145	GF	1317
1	Nup1	GJ	1317
1	Nup60	GK	1317
1	Mlp1	GO	1317
1	Mlp2	GP	1317
1	Nup84	GG	1076
1	Nup85	GL	1076
1	Nup120	GQ	1076

1	Nup133	GH	539
1	Nup145c	GI	539
1	Seh1	GM	539
1	Sec13	GN	539
1	Dyn2	GR	539
1	Nup82	GS	539
1	Nup159	GT	1875
1	Nsp1	GV	1875
1	Nic96	GX	1875
1	Nup49	GU	1679
1	Nup57	GW	1679
1	Nup157	GY	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(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
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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

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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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