Full wwPDB Integrative Structure Validation Report

November 05, 2019 -- 04:07 PM

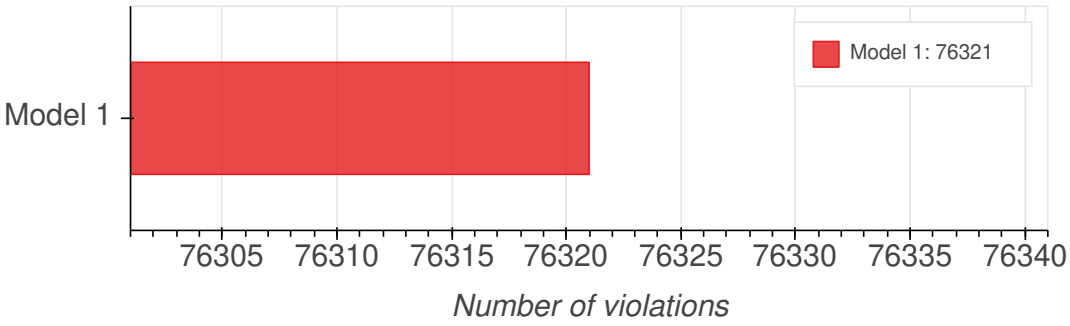
PDB ID	*PDBDEV00000010*
Molecule Name	Integrative structure and functional anatomy of a single spoke of a nuclear pore complex
Title	Integrative structure and functional anatomy of a nuclear pore complex.
Authors	Kim SJ;Fernandez-Martinez J;Nudelman I;Shi Y;Zhang W;Raveh B;Herricks T;Slaughter BD;Hogan 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 software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

Model quality: Excluded Volume Analysis



2. Ensemble information

This entry consists of 1 distinct ensemble.

Ensemble number	Ensemble name	Model ID	Number of models	Clustering method	Clustering feature	Cluster precision
1	Scaffold cluster 1	1	5	None	dRMSD	1.0

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 69 subunits in each model. A total of 65 datasets or restraints was used to build this entry. Each model is represented by 24 rigid bodies and 816 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled Scaffold cluster 1/None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	Nup84	A	726
1	2	1	Nup84	H	726
1	3	2	Nup85	B	744
1	4	2	Nup85	I	744
1	5	3	Nup120	C	1037
1	6	3	Nup120	J	1037
1	7	4	Nup133	D	1157
1	8	4	Nup133	K	1157
1	9	5	Nup145c	E	712
1	10	5	Nup145c	L	712
1	11	6	Seh1	F	349
1	12	6	Seh1	M	349
1	13	7	Sec13	G	297
1	14	7	Sec13	N	297
1	15	8	Dyn2	O	92

1	16	8	Dyn2	P	92
1	17	9	Nup82	Q	713
1	18	9	Nup82	R	713
1	19	10	Nup159	S	1460
1	20	10	Nup159	T	1460
1	21	11	Nsp1	U	823
1	22	11	Nsp1	V	823
1	23	11	Nsp1	X	823
1	24	11	Nsp1	AB	823
1	25	11	Nsp1	AF	823
1	26	11	Nsp1	AJ	823
1	27	12	Nic96	W	839
1	28	12	Nic96	AA	839
1	29	12	Nic96	AE	839
1	30	12	Nic96	AI	839
1	31	13	Nup49	Y	472
1	32	13	Nup49	AC	472
1	33	13	Nup49	AG	472
1	34	13	Nup49	AK	472
1	35	14	Nup57	Z	541
1	36	14	Nup57	AD	541
1	37	14	Nup57	AH	541
1	38	14	Nup57	AL	541
1	39	15	Nup157	AM	1391
1	40	15	Nup157	AQ	1391
1	41	16	Nup170	AN	1502
1	42	16	Nup170	AR	1502

1	43	17	Nup188	AO	1655
1	44	17	Nup188	AS	1655
1	45	18	Nup192	AP	1683
1	46	18	Nup192	AT	1683
1	47	19	Nup53	AU	475
1	48	19	Nup53	AZ	475
1	49	20	Nup59	AV	528
1	50	20	Nup59	BA	528
1	51	21	Ndc1	AW	655
1	52	21	Ndc1	BB	655
1	53	22	Pom34	AX	299
1	54	22	Pom34	BC	299
1	55	23	Pom152	AY	1337
1	56	23	Pom152	BD	1337
1	57	24	Nup100	BE	959
1	58	24	Nup100	BF	959
1	59	25	Nup116	BG	1113
1	60	25	Nup116	BH	1113
1	61	26	Nup42	BI	430
1	62	27	Gle1	BJ	538
1	63	28	Nup145	BK	1317
1	64	28	Nup145	BL	1317
1	65	29	Nup1	BM	1076
1	66	30	Nup60	BN	539
1	67	30	Nup60	BO	539
1	68	31	Mlp1	BP	1875
1	69	32	Mlp2	BQ	1679

3.3 Datasets used for modeling

There are 65 unique datasets used to build the models 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

4. Representation

This entry has only one representation and includes 24 rigid bodies and 816 flexible units.

Chain ID	***Rigid bodies***	***Non-rigid segments***
A	-	1-6, 7-20, 21-26, 27-80, 81-95, 96-126, 127-135, 136-364, 365-371, 372-483, 484-505, 506-562, 563-574, 575-726.
B	-	1-46, 47-126, 127-131, 132-230, 231-234, 235-436, 437-450, 451-492, 493-495, 496-544, 545-552, 553-560, 561-566, 567-585, 586-589, 590-597, 598-602, 603-612, 613-615, 616-634, 635-637, 638-655, 656-660, 661-675, 676-684, 685-699, 700-706, 707-719, 720-724, 725-744.

C	-	1-1, 2-29, 30-52, 53-305, 306-310, 311-711, 712-714, 715-726, 727-732, 733-746, 747-753, 754-766, 767-769, 770-781, 782-806, 807-818, 819-820, 821-833, 834-837, 838-853, 854-861, 862-879, 880-883, 884-895, 896-900, 901-913, 914-916, 917-931, 932-942, 943-955, 956-959, 960-971, 972-975, 976-987, 988-993, 994-1008, 1009-1024, 1025-1036, 1037-1037.
D	-	1-55, 56-78, 79-85, 86-125, 126-132, 133-144, 145-161, 162-184, 185-192, 193-200, 201-205, 206-249, 250-257, 258-480, 481-489, 490-763, 764-771, 772-1155, 1156-1157.
E	-	1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 551-553, 554-560, 561-565, 566-576, 577-586, 587-602, 603-611, 612-624, 625-630, 631-645, 646-653, 654-673, 674-680, 681-689, 690-702, 703-712.
F	-	1-248, 249-287, 288-346, 347-349.
G	-	1-9, 10-158, 159-165, 166-296, 297-297.
H	-	1-6, 7-20, 21-26, 27-80, 81-95, 96-126, 127-135, 136-364, 365-371, 372-483, 484-505, 506-562, 563-574, 575-726.
I	-	1-46, 47-126, 127-131, 132-230, 231-234, 235-436, 437-450, 451-492, 493-495, 496-544, 545-552, 553-560, 561-566, 567-585, 586-589, 590-597, 598-602, 603-612, 613-615, 616-634, 635-637, 638-655, 656-660, 661-675, 676-684, 685-699, 700-706, 707-719, 720-724, 725-744.

J	-	1-1, 2-29, 30-52, 53-305, 306-310, 311-711, 712-714, 715-726, 727-732, 733-746, 747-753, 754-766, 767-769, 770-781, 782-806, 807-818, 819-820, 821-833, 834-837, 838-853, 854-861, 862-879, 880-883, 884-895, 896-900, 901-913, 914-916, 917-931, 932-942, 943-955, 956-959, 960-971, 972-975, 976-987, 988-993, 994-1008, 1009-1024, 1025-1036, 1037-1037.
K	-	1-55, 56-78, 79-85, 86-125, 126-132, 133-144, 145-161, 162-184, 185-192, 193-200, 201-205, 206-249, 250-257, 258-480, 481-489, 490-763, 764-771, 772-1155, 1156-1157.
L	-	1-91, 92-99, 100-125, 126-144, 145-148, 149-550, 551-553, 554-560, 561-565, 566-576, 577-586, 587-602, 603-611, 612-624, 625-630, 631-645, 646-653, 654-673, 674-680, 681-689, 690-702, 703-712.
M	-	1-248, 249-287, 288-346, 347-349.
N	-	1-9, 10-158, 159-165, 166-296, 297-297.
O	-	1-6, 7-92.
P	-	1-6, 7-92.
Q	-	1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713.
R	-	1-6, 7-16, 17-22, 23-120, 121-122, 123-452, 453-521, 522-612, 613-624, 625-669, 670-677, 678-713.
S	-	1082-1116, 1117-1126, 1127-1210, 1211-1239, 1240-1265, 1266-1321, 1322-1331, 1332-1372, 1373-1381, 1382-1412, 1413-1428, 1429-1456, 1457-1460.

T	-	1082-1116, 1117-1126, 1127-1210, 1211-1239, 1240-1265, 1266-1321, 1322-1331, 1332-1372, 1373-1381, 1382-1412, 1413-1428, 1429-1456, 1457-1460.
U	-	601-636, 637-727, 728-741, 742-778, 779-787, 788-823.
V	-	601-636, 637-727, 728-741, 742-778, 779-787, 788-823.
W	20-56:Comparative model/None.	1-19, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839.
X	637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None.	601-636, 728-741, 779-787.
Y	270-359:Comparative model/None, 369-407:Comparative model/None, 433-472:Comparative model/None.	201-269, 360-368, 408-432.
Z	287-423:Comparative model/None, 433-476:Comparative model/None, 505-540:Comparative model/None.	201-286, 424-432, 477-504, 541-541.
AA	20-56:Comparative model/None.	1-19, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839.
AB	637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None.	601-636, 728-741, 779-787.
AC	270-359:Comparative model/None, 369-407:Comparative model/None, 433-472:Comparative model/None.	201-269, 360-368, 408-432.
AD	287-423:Comparative model/None, 433-476:Comparative model/None, 505-540:Comparative model/None.	201-286, 424-432, 477-504, 541-541.

AE	-	1-19, 20-56, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839.
AF	-	601-636, 637-727, 728-741, 742-778, 779-787, 788-823.
AG	-	201-269, 270-359, 360-368, 369-407, 408-432, 433-472.
AH	-	201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541.
AI	-	1-19, 20-56, 57-204, 205-360, 361-365, 366-374, 375-404, 405-444, 445-454, 455-515, 516-532, 533-747, 748-752, 753-835, 836-839.
AJ	-	601-636, 637-727, 728-741, 742-778, 779-787, 788-823.
AK	-	201-269, 270-359, 360-368, 369-407, 408-432, 433-472.
AL	-	201-286, 287-423, 424-432, 433-476, 477-504, 505-540, 541-541.
AM	-	1-87, 88-289, 290-300, 301-309, 310-338, 339-457, 458-480, 481-515, 516-534, 535-679, 680-703, 704-730, 731-743, 744-775, 776-785, 786-830, 831-835, 836-892, 893-899, 900-916, 917-920, 921-933, 934-943, 944-1016, 1017-1038, 1039-1141, 1142-1154, 1155-1390, 1391-1391.
AN	-	1-97, 98-299, 300-310, 311-319, 320-352, 353-471, 472-504, 505-537, 538-573, 574-717, 718-764, 765-791, 792-830, 831-862, 863-883, 884-916, 917-918, 919-930, 931-935, 936-992, 993-999, 1000-1016, 1017-1020, 1021-1033, 1034-1043, 1044-1116, 1117-1140, 1141-1191, 1192-1194, 1195-1243, 1244-1256, 1257-1502.

AO	-	1-11, 12-34, 35-39, 40-91, 92-100, 101-123, 124-130, 131-166, 167-173, 174-224, 225-255, 256-282, 283-287, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 608-619, 620-631, 632-785, 786-792, 793-889, 890-891, 892-1100, 1101-1118, 1119-1133, 1134-1156, 1157-1241, 1242-1246, 1247-1265, 1266-1275, 1276-1292, 1293-1302, 1303-1322, 1323-1331, 1332-1354, 1355-1382, 1383-1567, 1568-1592, 1593-1628, 1629-1632, 1633-1652, 1653-1655.
AP	-	1-362, 363-416, 417-574, 575-601, 602-798, 799-813, 814-849, 850-856, 857-953, 954-960, 961-1126, 1127-1136, 1137-1226, 1227-1233, 1234-1258, 1259-1271, 1272-1366, 1367-1370, 1371-1418, 1419-1420, 1421-1502, 1503-1510, 1511-1559, 1560-1583, 1584-1590, 1591-1596, 1597-1619, 1620-1622, 1623-1644, 1645-1650, 1651-1683.
AQ	-	1-87, 88-289, 290-300, 301-309, 310-338, 339-457, 458-480, 481-515, 516-534, 535-679, 680-703, 704-730, 731-743, 744-775, 776-785, 786-830, 831-835, 836-892, 893-899, 900-916, 917-920, 921-933, 934-943, 944-1016, 1017-1038, 1039-1141, 1142-1154, 1155-1390, 1391-1391.
AR	-	1-97, 98-299, 300-310, 311-319, 320-352, 353-471, 472-504, 505-537, 538-573, 574-717, 718-764, 765-791, 792-830, 831-862, 863-883, 884-916, 917-918, 919-930, 931-935, 936-992, 993-999, 1000-1016, 1017-1020, 1021-1033, 1034-1043, 1044-1116, 1117-1140, 1141-1191, 1192-1194, 1195-1243, 1244-1256, 1257-1502.

AS	-	1-11, 12-34, 35-39, 40-91, 92-100, 101-123, 124-130, 131-166, 167-173, 174-224, 225-255, 256-282, 283-287, 288-304, 305-317, 318-434, 435-438, 439-479, 480-492, 493-508, 509-514, 515-530, 531-550, 551-577, 578-583, 584-605, 606-607, 608-619, 620-631, 632-785, 786-792, 793-889, 890-891, 892-1100, 1101-1118, 1119-1133, 1134-1156, 1157-1241, 1242-1246, 1247-1265, 1266-1275, 1276-1292, 1293-1302, 1303-1322, 1323-1331, 1332-1354, 1355-1382, 1383-1567, 1568-1592, 1593-1628, 1629-1632, 1633-1652, 1653-1655.
AT	-	1-362, 363-416, 417-574, 575-601, 602-798, 799-813, 814-849, 850-856, 857-953, 954-960, 961-1126, 1127-1136, 1137-1226, 1227-1233, 1234-1258, 1259-1271, 1272-1366, 1367-1370, 1371-1418, 1419-1420, 1421-1502, 1503-1510, 1511-1559, 1560-1583, 1584-1590, 1591-1596, 1597-1619, 1620-1622, 1623-1644, 1645-1650, 1651-1683.
AU	-	1-247, 248-284, 285-303, 304-360, 361-475.
AV	-	1-265, 266-302, 303-345, 346-402, 403-528.
AW	-	1-655.
AX	-	1-299.
AY	-	1-378, 379-472, 473-519, 520-611, 612-615, 616-714, 715-721, 722-818, 819-823, 824-918, 919-930, 931-1026, 1027-1035, 1036-1141, 1142-1149, 1150-1229, 1230-1243, 1244-1337.
AZ	-	1-247, 248-284, 285-303, 304-360, 361-475.
BA	-	1-265, 266-302, 303-345, 346-402, 403-528.
BB	-	1-655.
BC	-	1-299.

BD	-	1-378, 379-472, 473-519, 520-611, 612-615, 616-714, 715-721, 722-818, 819-823, 824-918, 919-930, 931-1026, 1027-1035, 1036-1141, 1142-1149, 1150-1229, 1230-1243, 1244-1337.
BE	816-958:Comparative model/None.	551-815, 959-959.
BF	816-958:Comparative model/None.	551-815, 959-959.
BG	-	751-965, 966-1111, 1112-1113.
BH	-	751-965, 966-1111, 1112-1113.
BI	-	-
BJ	-	1-120.
BK	459-605:Experimental model/None.	201-458.
BL	459-605:Experimental model/None.	201-458.
BM	-	1-351.
BN	-	1-398.
BO	-	1-398.
BP	-	238-716.
BQ	-	215-690.

5. 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
2	1	Replica exchange monte carlo	Sampling	3000	False	True

3	1	Replica exchange monte carlo	Sampling	1000	False	True

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

6. Data quality

7. Model quality

7.1 Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

Models	*Excluded Volume Satisfaction*	*Number of violations*
1	99.98	76321

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model