

# Integrative Structure Validation Report

August 15, 2024 - 02:06 PM PDT

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


*Python-IHM Version 1.3*

*Integrative Modeling Validation Version 1.2*

PDB ID	9A8N
PDB-Dev ID	PDBDEV_00000387
Structure Title	Modeling of Yeast NPC basket
Structure Authors	Singh, D.; Soni, N.; Hutchings, J.; Echeverria, I.; Shaikh, F.; Duquette, M.; Suslov, S.; Li, Z.; van Eeuwen, T.; Molloy, K.; Shi, Y.; Wang, J.; Guo, Q.; Chait, B.T.; Fernandez-Martinez, J.; Rout, M.P.; Sali, A.; Villa, E.

*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](mailto:pdb-dev@mail.wwpdb.org)*

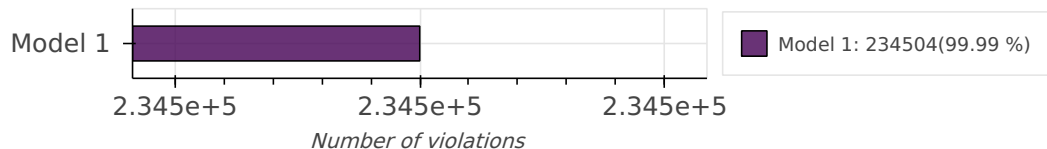
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the  symbol.*

*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. Number of plots is limited to 256.*

Model Quality: Excluded Volume Analysis



## Ensemble information ?

*This entry consists of 1 distinct ensemble(s).*

## Summary ?

*This entry consists of 1 unique models, with 168 subunits in each model. A total of 11 datasets or restraints were used to build this entry. Each model is represented by 912 rigid bodies and 1000 flexible or non-rigid units.*

## Entry composition ?

*There is 1 unique type of models in this entry. This model is titled Cluster 0/centroid-C8-symmetric.*

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Unknown MLP Protein	A	A	1875
1	2	1	Unknown MLP Protein	B	B	1875
1	3	1	Unknown MLP Protein	C	C	1875
1	4	1	Unknown MLP Protein	D	D	1875
1	5	1	Unknown MLP Protein	E	E	1875
1	6	1	Unknown MLP Protein	F	F	1875
1	7	1	Unknown MLP Protein	G	G	1875
1	8	1	Unknown MLP Protein	H	H	1875
1	9	1	Unknown MLP Protein	I	I	1875
1	10	1	Unknown MLP Protein	J	J	1875
1	11	1	Unknown MLP Protein	K	K	1875

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	12	1	Unknown MLP Protein	L	L	1875
1	13	1	Unknown MLP Protein	M	M	1875
1	14	1	Unknown MLP Protein	N	N	1875
1	15	1	Unknown MLP Protein	O	O	1875
1	16	1	Unknown MLP Protein	P	P	1875
1	17	2	Nucleoporin NUP1	Q	Q	1076
1	18	2	Nucleoporin NUP1	R	R	1076
1	19	2	Nucleoporin NUP1	S	S	1076
1	20	2	Nucleoporin NUP1	T	T	1076
1	21	2	Nucleoporin NUP1	U	U	1076
1	22	2	Nucleoporin NUP1	V	V	1076
1	23	2	Nucleoporin NUP1	W	W	1076
1	24	2	Nucleoporin NUP1	X	X	1076
1	25	3	Nucleoporin NUP2	Y	Y	720
1	26	3	Nucleoporin NUP2	Z	Z	720
1	27	3	Nucleoporin NUP2	AA	AA	720
1	28	3	Nucleoporin NUP2	AB	AB	720
1	29	3	Nucleoporin NUP2	AC	AC	720
1	30	3	Nucleoporin NUP2	AD	AD	720
1	31	3	Nucleoporin NUP2	AE	AE	720
1	32	3	Nucleoporin NUP2	AF	AF	720
1	33	3	Nucleoporin NUP2	AG	AG	720
1	34	3	Nucleoporin NUP2	AH	AH	720

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	35	3	Nucleoporin NUP2	AI	AI	720
1	36	3	Nucleoporin NUP2	AJ	AJ	720
1	37	3	Nucleoporin NUP2	AK	AK	720
1	38	3	Nucleoporin NUP2	AL	AL	720
1	39	3	Nucleoporin NUP2	AM	AM	720
1	40	3	Nucleoporin NUP2	AN	AN	720
1	41	4	Nucleoporin NUP60	AO	AO	539
1	42	4	Nucleoporin NUP60	AP	AP	539
1	43	4	Nucleoporin NUP60	AQ	AQ	539
1	44	4	Nucleoporin NUP60	AR	AR	539
1	45	4	Nucleoporin NUP60	AS	AS	539
1	46	4	Nucleoporin NUP60	AT	AT	539
1	47	4	Nucleoporin NUP60	AU	AU	539
1	48	4	Nucleoporin NUP60	AV	AV	539
1	49	4	Nucleoporin NUP60	AW	AW	539
1	50	4	Nucleoporin NUP60	AX	AX	539
1	51	4	Nucleoporin NUP60	AY	AY	539
1	52	4	Nucleoporin NUP60	AZ	AZ	539
1	53	4	Nucleoporin NUP60	BA	BA	539
1	54	4	Nucleoporin NUP60	BB	BB	539
1	55	4	Nucleoporin NUP60	BC	BC	539
1	56	4	Nucleoporin NUP60	BD	BD	539
1	57	5	Nucleoporin NUP120	BE	BE	1037

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	58	5	Nucleoporin NUP120	BF	BF	1037
1	59	5	Nucleoporin NUP120	BG	BG	1037
1	60	5	Nucleoporin NUP120	BH	BH	1037
1	61	5	Nucleoporin NUP120	BI	BI	1037
1	62	5	Nucleoporin NUP120	BJ	BJ	1037
1	63	5	Nucleoporin NUP120	BK	BK	1037
1	64	5	Nucleoporin NUP120	BL	BL	1037
1	65	5	Nucleoporin NUP120	BM	BM	1037
1	66	5	Nucleoporin NUP120	BN	BN	1037
1	67	5	Nucleoporin NUP120	BO	BO	1037
1	68	5	Nucleoporin NUP120	BP	BP	1037
1	69	5	Nucleoporin NUP120	BQ	BQ	1037
1	70	5	Nucleoporin NUP120	BR	BR	1037
1	71	5	Nucleoporin NUP120	BS	BS	1037
1	72	5	Nucleoporin NUP120	BT	BT	1037
1	73	6	Nucleoporin NUP85	BU	BU	744
1	74	6	Nucleoporin NUP85	BV	BV	744
1	75	6	Nucleoporin NUP85	BW	BW	744
1	76	6	Nucleoporin NUP85	BX	BX	744
1	77	6	Nucleoporin NUP85	BY	BY	744
1	78	6	Nucleoporin NUP85	BZ	BZ	744
1	79	6	Nucleoporin NUP85	CA	CA	744
1	80	6	Nucleoporin NUP85	CB	CB	744

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	81	6	Nucleoporin NUP85	CC	CC	744
1	82	6	Nucleoporin NUP85	CD	CD	744
1	83	6	Nucleoporin NUP85	CE	CE	744
1	84	6	Nucleoporin NUP85	CF	CF	744
1	85	6	Nucleoporin NUP85	CG	CG	744
1	86	6	Nucleoporin NUP85	CH	CH	744
1	87	6	Nucleoporin NUP85	CI	CI	744
1	88	6	Nucleoporin NUP85	CJ	CJ	744
1	89	7	Nucleoporin NUP145C	CK	CK	712
1	90	7	Nucleoporin NUP145C	CL	CL	712
1	91	7	Nucleoporin NUP145C	CM	CM	712
1	92	7	Nucleoporin NUP145C	CN	CN	712
1	93	7	Nucleoporin NUP145C	CO	CO	712
1	94	7	Nucleoporin NUP145C	CP	CP	712
1	95	7	Nucleoporin NUP145C	CQ	CQ	712
1	96	7	Nucleoporin NUP145C	CR	CR	712
1	97	7	Nucleoporin NUP145C	CS	CS	712
1	98	7	Nucleoporin NUP145C	CT	CT	712
1	99	7	Nucleoporin NUP145C	CU	CU	712
1	100	7	Nucleoporin NUP145C	CV	CV	712
1	101	7	Nucleoporin NUP145C	CW	CW	712
1	102	7	Nucleoporin NUP145C	CX	CX	712
1	103	7	Nucleoporin NUP145C	CY	CY	712

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	104	7	Nucleoporin NUP145C	CZ	CZ	712
1	105	8	Protein transport protein SEC13	DA	DA	297
1	106	8	Protein transport protein SEC13	DB	DB	297
1	107	8	Protein transport protein SEC13	DC	DC	297
1	108	8	Protein transport protein SEC13	DD	DD	297
1	109	8	Protein transport protein SEC13	DE	DE	297
1	110	8	Protein transport protein SEC13	DF	DF	297
1	111	8	Protein transport protein SEC13	DG	DG	297
1	112	8	Protein transport protein SEC13	DH	DH	297
1	113	8	Protein transport protein SEC13	DI	DI	297
1	114	8	Protein transport protein SEC13	DJ	DJ	297
1	115	8	Protein transport protein SEC13	DK	DK	297
1	116	8	Protein transport protein SEC13	DL	DL	297
1	117	8	Protein transport protein SEC13	DM	DM	297
1	118	8	Protein transport protein SEC13	DN	DN	297

<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	119	8	Protein transport protein SEC13	DO	DO	297
1	120	8	Protein transport protein SEC13	DP	DP	297
1	121	9	Nucleoporin SEH1	DQ	DQ	349
1	122	9	Nucleoporin SEH1	DR	DR	349
1	123	9	Nucleoporin SEH1	DS	DS	349
1	124	9	Nucleoporin SEH1	DT	DT	349
1	125	9	Nucleoporin SEH1	DU	DU	349
1	126	9	Nucleoporin SEH1	DV	DV	349
1	127	9	Nucleoporin SEH1	DW	DW	349
1	128	9	Nucleoporin SEH1	DX	DX	349
1	129	9	Nucleoporin SEH1	DY	DY	349
1	130	9	Nucleoporin SEH1	DZ	DZ	349
1	131	9	Nucleoporin SEH1	EA	EA	349
1	132	9	Nucleoporin SEH1	EB	EB	349
1	133	9	Nucleoporin SEH1	EC	EC	349
1	134	9	Nucleoporin SEH1	ED	ED	349
1	135	9	Nucleoporin SEH1	EE	EE	349
1	136	9	Nucleoporin SEH1	EF	EF	349
1	137	10	Nucleoporin NUP84	EG	EG	726
1	138	10	Nucleoporin NUP84	EH	EH	726
1	139	10	Nucleoporin NUP84	EI	EI	726
1	140	10	Nucleoporin NUP84	EJ	EJ	726



<b>Model ID</b>	<b>Subunit number</b>	<b>Subunit ID</b>	<b>Subunit name</b>	<b>Chain ID</b>	<b>Chain ID [auth]</b>	<b>Total residues</b>
1	141	10	Nucleoporin NUP84	EK	EK	726
1	142	10	Nucleoporin NUP84	EL	EL	726
1	143	10	Nucleoporin NUP84	EM	EM	726
1	144	10	Nucleoporin NUP84	EN	EN	726
1	145	10	Nucleoporin NUP84	EO	EO	726
1	146	10	Nucleoporin NUP84	EP	EP	726
1	147	10	Nucleoporin NUP84	EQ	EQ	726
1	148	10	Nucleoporin NUP84	ER	ER	726
1	149	10	Nucleoporin NUP84	ES	ES	726
1	150	10	Nucleoporin NUP84	ET	ET	726
1	151	10	Nucleoporin NUP84	EU	EU	726
1	152	10	Nucleoporin NUP84	EV	EV	726
1	153	11	Nucleoporin NUP133	EW	EW	1157
1	154	11	Nucleoporin NUP133	EX	EX	1157
1	155	11	Nucleoporin NUP133	EY	EY	1157
1	156	11	Nucleoporin NUP133	EZ	EZ	1157
1	157	11	Nucleoporin NUP133	FA	FA	1157
1	158	11	Nucleoporin NUP133	FB	FB	1157
1	159	11	Nucleoporin NUP133	FC	FC	1157
1	160	11	Nucleoporin NUP133	FD	FD	1157
1	161	11	Nucleoporin NUP133	FE	FE	1157
1	162	11	Nucleoporin NUP133	FF	FF	1157
1	163	11	Nucleoporin NUP133	FG	FG	1157

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	164	11	Nucleoporin NUP133	FH	FH	1157
1	165	11	Nucleoporin NUP133	FI	FI	1157
1	166	11	Nucleoporin NUP133	FJ	FJ	1157
1	167	11	Nucleoporin NUP133	FK	FK	1157
1	168	11	Nucleoporin NUP133	FL	FL	1157

### Datasets used for modeling ?

*There are 11 unique datasets used to build the models in this entry.*

ID	Dataset type	Database name	Data access code
7	Crosslinking-MS data	File	10.5281/zenodo.13131753
8	Crosslinking-MS data	File	10.5281/zenodo.13131753
1	De Novo model	File	10.5281/zenodo.13131753
2	De Novo model	File	10.5281/zenodo.13131753
3	De Novo model	File	10.5281/zenodo.13131753
4	De Novo model	File	10.5281/zenodo.13131753
6	Experimental model	File	10.5281/zenodo.13131753
10	3DEM volume	File	10.5281/zenodo.13131753
11	3DEM volume	File	10.5281/zenodo.13131753
5	Experimental model	PDB	7N84
9	3DEM volume	EMDB	EMD-44377

### Representation ?

*This entry has only one representation and includes 912 rigid bodies and 1000 flexible units.*

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
A	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
P	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
O	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
D	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
C	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
B	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
Q	1-32, 85-104, 106-123	33-84, 105-105, 124-335
X	1-32, 85-104, 106-123	33-84, 105-105, 124-335

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
R	1-32, 85-104, 106-123	33-84, 105-105, 124-335
BE	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BT	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BS	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BH	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BG	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BF	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
AO	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
BD	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
BC	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AR	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AQ	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AP	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
Y	83-136, 602-720	1-82, 137-601
AN	83-136, 602-720	1-82, 137-601
AM	83-136, 602-720	1-82, 137-601
AB	83-136, 602-720	1-82, 137-601
AA	83-136, 602-720	1-82, 137-601
Z	83-136, 602-720	1-82, 137-601
DQ	1-248, 288-346	249-287, 347-349

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
EF	1-248, 288-346	249-287, 347-349
EE	1-248, 288-346	249-287, 347-349
DT	1-248, 288-346	249-287, 347-349
DS	1-248, 288-346	249-287, 347-349
DR	1-248, 288-346	249-287, 347-349
CK	119-712	1-118
CZ	119-712	1-118
CY	119-712	1-118
CN	119-712	1-118
CM	119-712	1-118
CL	119-712	1-118
EG	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
EV	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
EU	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
EJ	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
EI	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
EH	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484- 505, 563-574
BU	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
CJ	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CI	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
BX	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
BW	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
BV	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
EW	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
FL	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
FK	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
EZ	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
EY	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
EX	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
E	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
F	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875

Chain ID	Rigid bodies	Non-rigid segments
G	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
H	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
I	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
J	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
K	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
L	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
M	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
N	71-183, 197-221, 239-281, 285-324, 340-371, 435-463, 535-570, 575-617, 622-668, 689-717, 745-773, 791-840, 844-893, 930-986, 990-1088, 1092-1127, 1143-1199, 1212-1251, 1254-1286, 1290-1339, 1343-1385, 1408-1457	1-70, 184-196, 222-238, 282-284, 325-339, 372-434, 464-534, 571-574, 618-621, 669-688, 718-744, 774-790, 841-843, 894-929, 987-989, 1089-1091, 1128-1142, 1200-1211, 1252-1253, 1287-1289, 1340-1342, 1386-1407, 1458-1875
S	1-32, 85-104, 106-123	33-84, 105-105, 124-335
T	1-32, 85-104, 106-123	33-84, 105-105, 124-335
U	1-32, 85-104, 106-123	33-84, 105-105, 124-335
V	1-32, 85-104, 106-123	33-84, 105-105, 124-335
W	1-32, 85-104, 106-123	33-84, 105-105, 124-335
AC	83-136, 602-720	1-82, 137-601
AD	83-136, 602-720	1-82, 137-601
AE	83-136, 602-720	1-82, 137-601
AF	83-136, 602-720	1-82, 137-601
AG	83-136, 602-720	1-82, 137-601
AH	83-136, 602-720	1-82, 137-601
AI	83-136, 602-720	1-82, 137-601
AJ	83-136, 602-720	1-82, 137-601
AK	83-136, 602-720	1-82, 137-601
AL	83-136, 602-720	1-82, 137-601



<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
AS	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AT	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AU	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AV	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AW	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AX	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AY	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
AZ	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
BA	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
BB	27-47, 91-104, 106-119, 121-140, 142-162	1-26, 48-90, 105-105, 120-120, 141-141, 163-398, 505-539
BI	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BJ	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BK	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BL	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BM	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BN	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BO	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BP	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
BQ	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BR	1-29, 53-305, 311-711, 714-1036	30-52, 306-310, 712-713, 1037-1037
BY	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
BZ	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CA	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
CB	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CC	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
CD	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CE	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
CF	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CG	47-126, 132-230, 235-436, 451-744	1-46, 127-131, 231-234, 437-450
CH	47-126, 132-230, 235-436, 451-739	1-46, 127-131, 231-234, 437-450, 740-744
CO	119-712	1-118
CP	119-712	1-118
CQ	119-712	1-118
CR	119-712	1-118
CS	119-712	1-118
CT	119-712	1-118
CU	119-712	1-118
CV	119-712	1-118
CW	119-712	1-118
CX	119-712	1-118
DA	8-157, 170-293	1-7, 158-169, 294-297

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
DB	8-157, 170-293	1-7, 158-169, 294-297
DC	8-157, 170-293	1-7, 158-169, 294-297
DD	8-157, 170-293	1-7, 158-169, 294-297
DE	8-157, 170-293	1-7, 158-169, 294-297
DF	8-157, 170-293	1-7, 158-169, 294-297
DG	8-157, 170-293	1-7, 158-169, 294-297
DH	8-157, 170-293	1-7, 158-169, 294-297
DI	8-157, 170-293	1-7, 158-169, 294-297
DJ	8-157, 170-293	1-7, 158-169, 294-297
DK	8-157, 170-293	1-7, 158-169, 294-297
DL	8-157, 170-293	1-7, 158-169, 294-297
DM	8-157, 170-293	1-7, 158-169, 294-297
DN	8-157, 170-293	1-7, 158-169, 294-297
DO	8-157, 170-293	1-7, 158-169, 294-297
DP	8-157, 170-293	1-7, 158-169, 294-297
DU	1-248, 288-346	249-287, 347-349
DV	1-248, 288-346	249-287, 347-349
DW	1-248, 288-346	249-287, 347-349
DX	1-248, 288-346	249-287, 347-349
DY	1-248, 288-346	249-287, 347-349
DZ	1-248, 288-346	249-287, 347-349
EA	1-248, 288-346	249-287, 347-349
EB	1-248, 288-346	249-287, 347-349

<b>Chain ID</b>	<b>Rigid bodies</b>	<b>Non-rigid segments</b>
EC	1-248, 288-346	249-287, 347-349
ED	1-248, 288-346	249-287, 347-349
EK	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EL	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EM	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EN	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EO	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EP	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
EQ	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
ER	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
ES	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
ET	7-20, 27-80, 96-126, 136-364, 372-483, 506-562, 575-726	1-6, 21-26, 81-95, 127-135, 365-371, 484-505, 563-574
FA	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
FB	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
FC	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157

Chain ID	Rigid bodies	Non-rigid segments
FD	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
FE	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
FF	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
FG	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
FH	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157
FI	63-183, 198-480, 490-763, 772-1155	1-62, 184-197, 481-489, 764-771, 1156-1157
FJ	56-77, 86-125, 133-144, 162-184, 193-200, 206-249, 258-480, 490-763, 772-1155	1-55, 78-85, 126-132, 145-161, 185-192, 201-205, 250-257, 481-489, 764-771, 1156-1157

## Methodology and software

*This entry is a result of 1 distinct protocol(s).*

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	1000	False	True
2	1	Replica exchange monte carlo	Sampling	None	15467933	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.19.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
3	COCONUT	1.0.0	Coiled-coil model building	<a href="https://github.com/neeleshsoni21/COCONUT">https://github.com/neeleshsoni21/COCONUT</a>
2	Integrative Modeling Platform (IMP)	2.19.0	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>

### Data quality ?

#### Crosslinking-MS

Validation for this section is under development.

#### 3DEM volume

Validation for this section is under development.

### Model quality ?

For models with atomic structures, molprobit analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

#### Excluded volume satisfaction ?

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

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.99	234504.0

### Fit of model to data used for modeling ?

#### Crosslinking-MS

Validation for this section is under development.

#### 3DEM volume

Validation for this section is under development.

## Fit of model to data used for validation

Validation for this section is under development.

---

### *Acknowledgements*

*Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*