Full wwPDB Integrative Structure Validation Report

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PDB ID	***PDBDEV00000016***
Molecule Name	Integrative structure-function mapping of the nucleoporin Nup133
Title	Integrative structure-function mapping of the nucleoporin Nup133 suggests a conserved mechanism for membrane anchoring of the nuclear pore complex.
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The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

2. Ensemble information

This entry consists of 0 distinct ensemble.

3. Model composition

3.1 Summary

This entry consists of 4 unique models, with 1 subunits in each model. A total of 56 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

3.2 Entry composition

There are 4 unique types of models in this entry.These models are titled None/None, None/None, None/None, None/None respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	Nup133	A	1166
2	1	1	Nup133	A	1166
3	1	1	Nup133	A	1166
4	1	1	Nup133	A	1166

3.3 Datasets used for modeling

There are 56 unique datasets used to build the models in this entry.

ID	*Dataset type*	*Database name*	*Data access code*
1	SAS data	Not listed	None
2	SAS data	Not listed	None
3	SAS data	Not listed	None
4	SAS data	Not listed	None
5	SAS data	Not listed	None
6	SAS data	Not listed	None
7	SAS data	Not listed	None
8	SAS data	Not listed	None
9	SAS data	Not listed	None
10	SAS data	Not listed	None
11	SAS data	Not listed	None

12	SAS data	Not listed	None
13	SAS data	Not listed	None
14	SAS data	Not listed	None
15	SAS data	Not listed	None
16	SAS data	Not listed	None
17	SAS data	Not listed	None
18	SAS data	Not listed	None
19	SAS data	Not listed	None
20	2DEM class average	Not listed	None
21	2DEM class average	Not listed	None
22	2DEM class average	Not listed	None
23	2DEM class average	Not listed	None
24	2DEM class average	Not listed	None
25	2DEM class average	Not listed	None
26	2DEM class average	Not listed	None
27	2DEM class average	Not listed	None
28	2DEM class average	Not listed	None
29	2DEM class average	Not listed	None
30	2DEM class average	Not listed	None
31	2DEM class average	Not listed	None
32	2DEM class average	Not listed	None
33	2DEM class average	Not listed	None
34	2DEM class average	Not listed	None
35	2DEM class average	Not listed	None
36	2DEM class average	Not listed	None
37	2DEM class average	Not listed	None
38	2DEM class average	Not listed	None

39	2DEM class average	Not listed	None
40	2DEM class average	Not listed	None
41	2DEM class average	Not listed	None
42	2DEM class average	Not listed	None
43	CX-MS data	Not listed	None
44	Experimental model	PDB	3I4R
45	Experimental model	PDB	3KFO
46	Experimental model	PDB	4Q9T
47	Experimental model	PDB	2JO8
48	Experimental model	PDB	2QIW
49	Experimental model	PDB	3CIG
50	Experimental model	PDB	2ELO
51	Experimental model	PDB	3GUZ
52	Experimental model	PDB	2CIW
53	Experimental model	PDB	1A92
54	Experimental model	PDB	1GDJ
55	Experimental model	PDB	1X4O
56	Comparative model	Not listed	None

4. Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units.

Chain ID	***Rigid bodies***	***Non-rigid segments***
A	-	1-1166.

5. Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	AllosMod	MD-based conformational sampling	7000	False	False
2	1	MES	Minimal Ensemble Search	4	True	False

There are 6 software packages reported in this entry.

ID	Software name	Software version	Software classification
1	HHpred	2.0.16	protein homology detection
2	PSIPRED	4.0	secondary structure prediction
3	DISOPRED	3	disorder prediction
4	Integrative Modeling Platform (IMP)	2.2	integrative model building
5	MODELLER	9.13	comparative modeling
6	AllosMod	None	sampling

6. Data quality

7. Model quality

7.1 Standard geometry

There are 5976 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
CE1--HE1	1.079	0.93	63
CD2--HD2	1.079	0.93	63
NZ--HZ3	1.039	0.89	17

CE2--HE2	1.079	0.93	57
CE3--HE3	1.079	0.93	7
CZ--HZ	1.079	0.93	47
NZ--HZ2	1.039	0.89	17
N--H2	1.041	0.89	1
CD1--HD1	1.079	0.93	65
NZ--HZ1	1.039	0.89	17
CH2--HH2	1.079	0.93	7
N--H3	1.04	0.89	1
CZ2--HZ2	1.08	0.93	7
CZ3--HZ3	1.08	0.93	7
N--H1	1.04	0.89	1
CG2--HG21	1.11	0.97	203
CD1--HD12	1.11	0.97	151
CG2--HG23	1.11	0.97	203
CD2--HD21	1.11	0.97	101
CG--HG3	1.11	0.97	147
CG1--HG12	1.11	0.97	149
CB--HB2	1.11	0.97	487
CB--HB	1.11	0.97	203
CD2--HD22	1.11	0.97	101
CG--HG	1.11	0.97	101
CB--HB3	1.11	0.97	481
CG1--HG11	1.11	0.97	99
CD1--HD13	1.11	0.97	151
CD--HD3	1.11	0.97	71
CG1--HG13	1.11	0.97	149

CB--HB1	1.11	0.97	103
CG--HG2	1.11	0.97	147
CG2--HG22	1.11	0.97	203
CD2--HD23	1.11	0.97	101
CD1--HD11	1.11	0.97	151
CE--HE3	1.11	0.97	51
CE--HE1	1.11	0.97	33
CD--HD2	1.11	0.97	71
CE--HE2	1.11	0.97	51
NH2--HH22	0.999	0.86	21
ND2--HD22	0.999	0.86	11
NE--HE	0.999	0.86	21
NH1--HH11	0.999	0.86	21
NH2--HH21	0.999	0.86	21
NE2--HE22	0.999	0.86	27
NE2--HE21	0.999	0.86	27
ND2--HD21	1	0.86	11
NH1--HH12	0.999	0.86	21
ND1--HD1	0.999	0.86	5
N--H	0.996	0.86	717
N--HN	0.996	0.86	5
SG--HG	1.325	1.2	1
OG--HG	0.959	0.84	33
OH--HH	0.959	0.84	9
OG1--HG1	0.959	0.84	53
NE1--HE1	0.976	0.86	7
CA--HA3	1.079	0.97	65

CA--HA	1.079	0.97	691
CA--HA2	1.079	0.97	65

There are 147 angle outliers in this entry.

Angle type	*Observed angle (°)*	*Ideal angle (°)*	*Number of outliers*
CA-CB-HB3	96.673	109	6
CB-CA-HA	96.154	109	5
HD21-CD2-HD23	97.398	110	2
NE2-CD2-HD2	113.697	126.4	1
CB-CG2-HG23	97.357	110	2
HG2-CG-HG3	96.297	110	2
CG-CB-HB2	120.468	108	3
C-N-H	112.176	124.3	30
N-CA-HA	97.676	110	2
HE2-CE-HE3	94.424	110	0
HB2-CB-HB3	97.713	110	7
HB1-CB-HB3	122.02	110	3
HD2-CD-HD3	94.615	110	0
CA-N-HN	129.327	114	0
HG12-CG1-HG13	97.549	110	2
CA-N-H	126.007	114	4
HD11-CD1-HD13	97.104	110	2
N-CA-HA3	97.28	110	1
CB-OG-HG	96.486	110	1
HB1-CB-HB2	97.982	110	1
N-CA-HA2	97.152	110	1
C-CA-HA	96.748	109	3
HG21-CG2-HG22	96.639	109	1

CD-CG-HG2	120.961	108	1
CE-NZ-HZ3	96.018	110	0
CB-CG2-HG21	122.855	110	1
HD11-CD1-HD12	96.739	110	1
HZ1-NZ-HZ2	95.3	109	0
CB-CG1-HG11	122.634	109	0
CA-CB-HB2	96.806	109	2
CB-OG1-HG1	97.762	110	3
HG21-CG2-HG23	97.538	110	2
C-CA-HA2	96.238	109	1
CD1-CG-HG	121.29	108	0
CB-CG1-HG12	95.736	109	0
CB-CG1-HG13	122.191	109	0
HG22-CG2-HG23	97.663	110	1
CB-CG-HG2	122.044	109	0
CG-CD2-HD23	121.948	109	0
CA-CB-HB	96.108	109	0
CG-CD1-HD12	121.846	109	0
CG-CD2-HD22	121.624	109	1
CB-CG-HG3	96.195	109	0
CG-CD2-HD21	121.761	109	0
HD21-CD2-HD22	97.293	110	0
CZ-NH2-HH21	107.301	120	0
HG11-CG1-HG12	97.312	110	0
CG-CB-HB3	95.557	108	1
CG1-CD1-HD12	121.356	109	0

CG1-CB-HB	96.815	109	0
SD-CE-HE2	121.147	109	0
CD-CG-HG3	120.046	108	0
CG-CD2-HD2	138.433	126.4	0
N-CD-HD2	121.015	109	0

7.2 Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	*Clash score*	*Number of clashes*
Model 1	0.86	10

All 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

7.3 Torsion angles

7.3.1 Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation wasanalysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	754	703	41	10

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:7	ASN
1	A:56	GLY
1	A:132	PRO
1	A:156	PRO
1	A:163	PRO
1	A:190	GLY

1	A:236	ILE
1	B:183	VAL
1	B:236	ILE
1	B:304	GLN

7.3.2 Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	*Analyzed*	*Favored*	*Allowed*	*Outliers*
1	594	536	41	17

Detailed list of outliers are tabulated below.

Model ID	*Chain and res ID*	*Residue type*
1	A:65	THR
1	A:73	THR
1	A:84	LEU
1	A:94	LEU
1	A:111	PRO
1	A:132	PRO
1	A:158	VAL
1	A:193	PRO
1	A:207	THR
1	A:280	THR
1	B:37	PRO
1	B:130	GLN
1	B:138	ASN
1	B:169	ILE
1	B:242	THR

1	B:284	ARG
1	B:347	LEU

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model