



Full wwPDB Integrative Structure Validation Report

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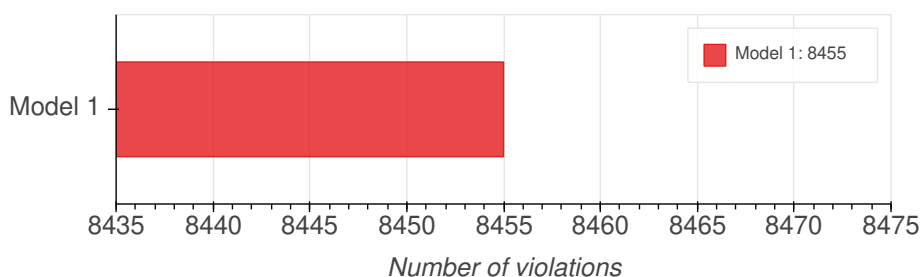
PDB ID	PDBDEV00000020
Molecule Name	Structure of the <i>S. cerevisiae</i> nuclear pore complex cytoplasmic mRNA export platform, Nup82
Title	Structure and Function of the Nuclear Pore Complex Cytoplasmic mRNA Export Platform.
Authors	Fernandez-Martinez J;Kim SJ;Shi Y;Upla P;Pellarin R;Gagnon M;Chemmmama IE;Wang J;Nudelman I;Zhang W;Williams R;Rice WJ;Stokes DL;Zenklusen D;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	Cluster 0	1	370	None	dRMSD	9.0

3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 10 subunits in each model. A total of 37 datasets or restraints was

used to build this entry. Each model is represented by 38 rigid bodies and 42 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry. This model is titled Cluster 0/None respectively.

<i>Model ID</i>	<i>Subunit number</i>	<i>Subunit ID</i>	<i>Subunit name</i>	<i>Chain ID</i>	<i>Total residues</i>
1	1	1	Dyn2	A	92
1	2	1	Dyn2	B	92
1	3	2	Nup82	C	713
1	4	2	Nup82	D	713
1	5	3	Nup159	E	1460
1	6	3	Nup159	F	1460
1	7	4	Nsp1	G	823
1	8	4	Nsp1	H	823
1	9	5	Nup116	I	1113
1	10	5	Nup116	J	1113

3.3 Datasets used for modeling

There are 37 unique datasets used to build the models in this entry.

<i>ID</i>	<i>Dataset type</i>	<i>Database name</i>	<i>Data access code</i>
1	Experimental model	PDB	4DS1
2	Experimental model	PDB	3PBP
3	Experimental model	PDB	5CWS
4	Comparative model	Not listed	None
5	Comparative model	Not listed	None
6	Comparative model	Not listed	None
7	Comparative model	Not listed	None
8	Comparative model	Not listed	None
9	Comparative model	Not listed	None
10	Experimental model	PDB	1XIP
11	CX-MS data	Not listed	None
12	CX-MS data	Not listed	None
13	CX-MS data	Not listed	None
14	2DEM class average	Not listed	None

15	2DEM class average	Not listed	None
16	2DEM class average	Not listed	None
17	2DEM class average	Not listed	None
18	2DEM class average	Not listed	None
19	2DEM class average	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	SAS data	Not listed	None
36	SAS data	Not listed	None
37	SAS data	Not listed	None

4. Representation

This entry has only one representation and includes 38 rigid bodies and 42 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
A	7-92:Experimental model/4DS1.	1-6.
B	7-92:Experimental model/4DS1.	1-6.

C	7-16:Experimental model/3PBP, 23-120:Experimental model/3PBP, 123-452:Experimental model/3PBP, 522-612:Comparative model/None, 625-669:Comparative model/None, 678-713:Comparative model/None.	1-6, 17-22, 121-122, 453-521, 613-624, 670-677.
D	7-16:Experimental model/3PBP, 23-120:Experimental model/3PBP, 123-452:Experimental model/3PBP, 522-612:Comparative model/None, 625-669:Comparative model/None, 678-713:Comparative model/None.	1-6, 17-22, 121-122, 453-521, 613-624, 670-677.
E	2-347:Experimental model/1XIP, 362-381:Experimental model/1XIP, 1117-1126:Experimental model/4DS1, 1211-1239:Comparative model/None, 1266-1321:Comparative model/None, 1332-1372:Comparative model/None, 1382-1412:Comparative model/None, 1429-1456:Experimental model/3PBP.	1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460.
F	2-347:Experimental model/1XIP, 362-381:Experimental model/1XIP, 1117-1126:Experimental model/4DS1, 1211-1239:Comparative model/None, 1266-1321:Comparative model/None, 1332-1372:Comparative model/None, 1382-1412:Comparative model/None, 1429-1456:Experimental model/3PBP.	1-1, 348-361, 382-1116, 1127-1210, 1240-1265, 1322-1331, 1373-1381, 1413-1428, 1457-1460.
G	637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None.	1-636, 728-741, 779-787.
H	637-727:Comparative model/None, 742-778:Comparative model/None, 788-823:Comparative model/None.	1-636, 728-741, 779-787.
I	966-1111:Experimental model/3PBP.	1-965, 1112-1113.
J	966-1111:Experimental model/3PBP.	1-965, 1112-1113.

5. Methodology and software

<i>Step number</i>	<i>Protocol ID</i>	<i>Method name</i>	<i>Method type</i>	<i>Number of computed models</i>	<i>Multi state modeling</i>	<i>Multi scale modeling</i>
1	1	Replica exchange monte carlo	Sampling	1000	False	True
2	1	Replica exchange monte carlo	Sampling	1350000	False	True
3	1	Replica exchange monte carlo	Sampling	10000	False	True

There are 9 software packages reported in this entry.

<i>ID</i>	<i>Software name</i>	<i>Software version</i>	<i>Software classification</i>	<i>Software location</i>
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.org
3	HHpred	2.0.16	protein homology detection	https://toolkit.tuebingen.mpg.de/
4	PSIPRED	4.0	secondary structure prediction	http://bioinf.cs.ucl.ac.uk/psipred/
5	DISOPRED	3	disorder prediction	http://bioinf.cs.ucl.ac.uk/psipred/?disopred=1
6	DomPred	None	domain prediction	http://bioinf.cs.ucl.ac.uk/psipred/?dompred=1
7	COILS/PCOILS	None	coiled-coil prediction	https://toolkit.tuebingen.mpg.de/
8	Multicoil2	None	coiled-coil prediction	http://groups.csail.mit.edu/cb/multicoil2.cgi
9	MODELLER	9.15	comparative modeling	https://salilab.org/modeller/

6. Data quality

7. Model quality

7.1 Excluded volume satisfaction

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

<i>Models</i>	<i>Excluded Volume Satisfaction</i>	<i>Number of violations</i>
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1	99.84	8455
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8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model
