



# Full wwPDB Integrative Structure Validation Report

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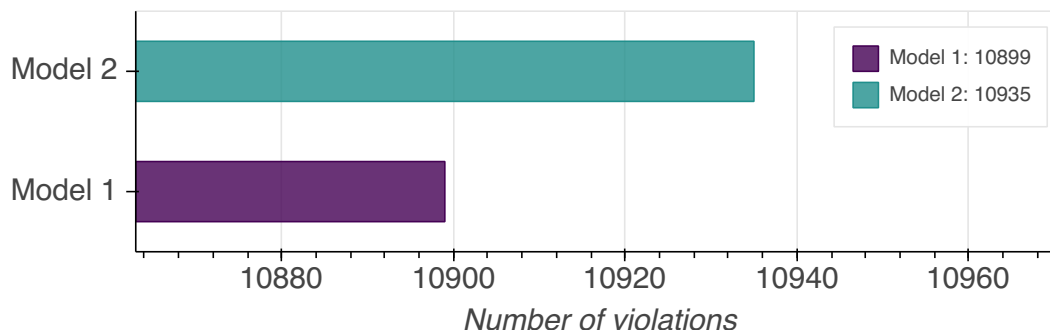
The following software were used in the production of this report:

*Integrative Modeling Validation Package : Version 1.0*

| PDB ID        | PDBDEV_00000001   |
|---------------|---|
| Molecule Name | Structure of the Nup84 sub-complex of the Nuclear Pore Complex  |
| Title         | Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptameric module from the nuclear pore complex. |
| Authors       | Shi Y;Fernandez-Martinez J;Tjioe E;Pellarin R;Kim SJ;Williams R;Schneidman-Duhovny D;Sali A;Rout MP;Chait BT  |

## Overall quality

### Model quality: Excluded Volume Analysis



### Ensemble information

*This entry consists of 2 distinct ensembles.*

### Entry composition

*There are 2 unique types of models in this entry. These models are titled Cluster 1/Best scoring model, Cluster 2/Best scoring model respectively.*

| Model ID | Subunit number | Subunit ID | Subunit name | Chain ID | Total residues |
|----------|----------------|------------|--------------|----------|----------------|
| 1        | 1              | 1          | Nup84        | A        | 726            |
| 1        | 2              | 2          | Nup85        | B        | 744            |
| 1        | 3              | 3          | Nup120       | C        | 1037           |
| 1        | 4              | 4          | Nup133       | D        | 1157           |
| 1        | 5              | 5          | Nup145c      | E        | 712            |
| 1        | 6              | 6          | Seh1         | F        | 349            |
| 1        | 7              | 7          | Sec13        | G        | 297            |
| 2        | 1              | 1          | Nup84        | A        | 726            |
| 2        | 2              | 2          | Nup85        | B        | 744            |
| 2        | 3              | 3          | Nup120       | C        | 1037           |
| 2        | 4              | 4          | Nup133       | D        | 1157           |
| 2        | 5              | 5          | Nup145c      | E        | 712            |
| 2        | 6              | 6          | Seh1         | F        | 349            |
| 2        | 7              | 7          | Sec13        | G        | 297            |

### 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    | 5000                      | False                | True                 |

## Data quality

### Model quality

#### Excluded volume satisfaction

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

| Models | Excluded Volume Satisfaction | Number of violations |
|--------|------------------------------|----------------------|
| 1      | 99.88                        | 10899.0              |
| 2      | 99.88                        | 10935.0              |

### Fit of model to data used for modeling

### Fit of model to data not used for modeling

### Uncertainty of data and model

