



Full wwPDB Integrative Structure Validation Report

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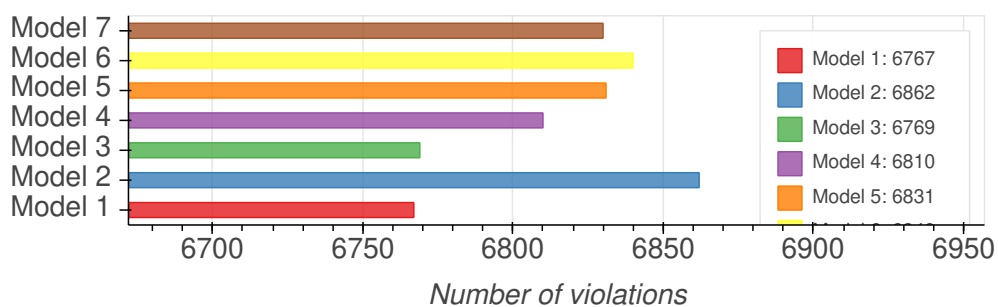
PDB ID	PDBDEV000000X
Molecule Name	Integrative structure of the human CSN complex
Title	Structural characterization by cross-linking reveals the detailed architecture of a coatomer-related heptameric module from the nuclear pore complex.
Authors	Shi Y;Fernandez-Martinez J;Tjioe E;Pellarin R;Kim SJ;Williams R;Schneidman-Duhovny D;Sali A;Rout MP;Chait BT

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 7 distinct ensembles.

Ensemble number	Ensemble name	Model ID	Number of models	Clustering method	Clustering feature	Cluster precision
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1	Ensemble generated using BMSO+DHSD+DSSO datasets in state State_0		54702	None	dRMSD	16.0
2	Ensemble generated using BMSO+DHSD datasets in state State_0	2	132407	None	dRMSD	22.0
3	Ensemble generated using DHSD+DSSO datasets in state State_0	3	98186	None	dRMSD	24.0
4	Ensemble generated using BMSO+DSSO datasets in state State_0	4	87368	None	dRMSD	27.0
5	Ensemble generated using DSSO datasets in state State_0	5	243067	None	dRMSD	27.0
6	Ensemble generated using DHSD datasets in state State_0	6	312515	None	dRMSD	29.0
7	Ensemble generated using BMSO datasets in state State_0	7	357350	None	dRMSD	37.0

3. Model composition

3.1 Summary

This entry consists of 7 unique models, with 8 subunits in each model. A total of 10 datasets or restraints was used to build this entry. Each model is represented by 23 rigid bodies and 28 flexible or non-rigid units.

3.2 Entry composition

There are 7 unique types of models in this entry. These models are titled Ensemble generated using BMSO+DHSO+DSSO datasets in state State_0/None, Ensemble generated using BMSO+DHSO datasets in state State_0/None, Ensemble generated using DHSO+DSSO datasets in state State_0/None, Ensemble generated using BMSO+DSSO datasets in state State_0/None, Ensemble generated using DSSO datasets in state State_0/None, Ensemble generated using DHSO datasets in state State_0/None, Ensemble generated using BMSO datasets in state State_0/None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	CSN1	A	491
1	2	2	CSN2	B	443
1	3	3	CSN3	C	423
1	4	4	CSN4	D	406
1	5	5	CSN5	E	334
1	6	6	CSN6	F	327
1	7	7	CSN7	G	264
1	8	8	CSN8	H	209
2	1	1	CSN1	A	491
2	2	2	CSN2	B	443
2	3	3	CSN3	C	423
2	4	4	CSN4	D	406
2	5	5	CSN5	E	334
2	6	6	CSN6	F	327
2	7	7	CSN7	G	264
2	8	8	CSN8	H	209
3	1	1	CSN1	A	491
3	2	2	CSN2	B	443
3	3	3	CSN3	C	423
3	4	4	CSN4	D	406
3	5	5	CSN5	E	334
3	6	6	CSN6	F	327
3	7	7	CSN7	G	264

3	8	8	CSN8	H	209
4	1	1	CSN1	A	491
4	2	2	CSN2	B	443
4	3	3	CSN3	C	423
4	4	4	CSN4	D	406
4	5	5	CSN5	E	334
4	6	6	CSN6	F	327
4	7	7	CSN7	G	264
4	8	8	CSN8	H	209
5	1	1	CSN1	A	491
5	2	2	CSN2	B	443
5	3	3	CSN3	C	423
5	4	4	CSN4	D	406
5	5	5	CSN5	E	334
5	6	6	CSN6	F	327
5	7	7	CSN7	G	264
5	8	8	CSN8	H	209
6	1	1	CSN1	A	491
6	2	2	CSN2	B	443
6	3	3	CSN3	C	423
6	4	4	CSN4	D	406
6	5	5	CSN5	E	334
6	6	6	CSN6	F	327
6	7	7	CSN7	G	264
6	8	8	CSN8	H	209
7	1	1	CSN1	A	491
7	2	2	CSN2	B	443
7	3	3	CSN3	C	423
7	4	4	CSN4	D	406

7	5	5	CSN5	E	334
7	6	6	CSN6	F	327
7	7	7	CSN7	G	264
7	8	8	CSN8	H	209

3.3 Datasets used for modeling

There are 10 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	Comparative model	Not listed	None
2	Experimental model	PDB	4D10
3	Experimental model	Not listed	None
4	Comparative model	Not listed	None
5	CX-MS data	Not listed	None
6	CX-MS data	Not listed	None
7	CX-MS data	Not listed	None
8	CX-MS data	Not listed	None
9	CX-MS data	Not listed	None
10	CX-MS data	Not listed	None

4. Representation

This entry has only one representation and includes 23 rigid bodies and 28 flexible units.

<i>Chain ID</i>	<i>Rigid bodies</i>	<i>Non-rigid segments</i>
A	44-107:Comparative model/None, 128-227:Comparative model/None, 246-426:Comparative model/None, 431-462:Comparative model/None.	1-43, 108-127, 228-245, 427-430, 463-491.
B	30-179:Experimental model/4D10, 192-289:Experimental model/4D10, 308-397:Experimental model/4D10, 417-443:Experimental model/4D10.	1-29, 180-191, 290-307, 398-416.

C	3-163:Experimental model/4D10, 177-361:Experimental model/4D10, 368- 401:Experimental model/4D10.	1-2, 164-176, 362-367, 402-423.
D	3-131:Experimental model/4D10, 139-361:Experimental model/4D10, 365- 406:Experimental model/4D10.	1-2, 132-138, 362-364.
E	25-283:Experimental model/4D10, 296- 333:Experimental model/4D10.	1-24, 284-295, 334-334.
F	29-207:Experimental model/4D10, 215- 267:Experimental model/4D10, 271-316:Experimental model/4D10.	1-28, 208-214, 268-270, 317-327.
G	8-158:Comparative model/None, 163-212:Comparative model/None.	1-7, 159-162, 213-264.
H	11-164:Experimental model/4D10, 194- 209:Experimental model/4D10.	1-10, 165-193.

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	5250000	False	True

There are 3 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	IMP PMI module	20191107.develop.2640aae65c	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	20191107.develop.2640aae65c	integrative model building	https://integrativemodeling.org
3	MODELLER	SVN	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>
1	99.79	6767.0
2	99.78	6862.0
3	99.79	6769.0
4	99.79	6810.0
5	99.78	6831.0
6	99.78	6840.0
7	99.78	6830.0

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model
