Full RCSB Integrative Structure Validation Report

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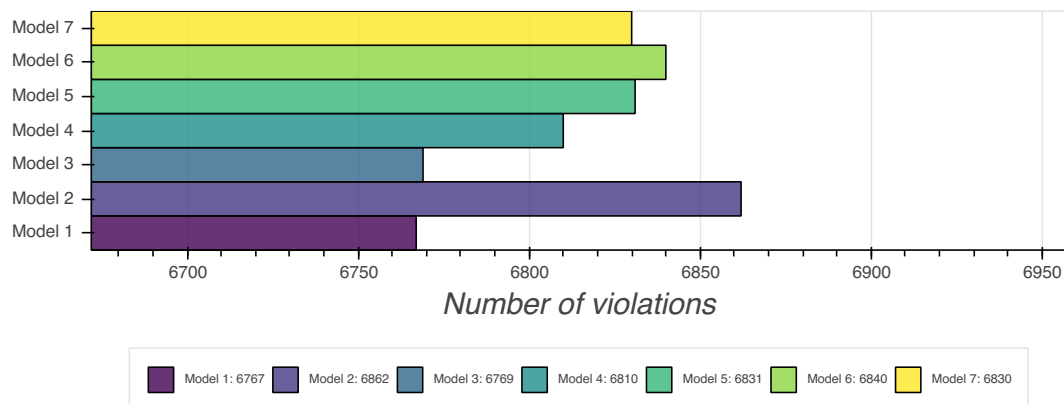
The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000037
Molecule Name	Integrative structure of the canonical human COP9 Signalosome
Title	Structural Dynamics of the Human COP9 Signalosome Revealed by an Integrated Approach
Authors	Gutierrez C;Chemmama IE;Mao H;Yu C;Echeverria I;Block S;Rychnovsky SD;Zheng N;Sali A;Huang L

Overall quality

Model quality: Excluded Volume Analysis

Number of violations

Model 1: 6767 Model 2: 6862 Model 3: 6769 Model 4: 6810 Model 5: 6831 Model 6: 6840 Model 7: 6830

Ensemble information

This entry consists of 7 distinct ensembles.

Entry composition

There are 7 unique types of models in this entry.These models are titled Cluster 0BMSO+DHSO+DSSO in state State_0/None, Cluster 0BMSO+DHSO in state State_0/None, Cluster 0DHSO+DSSO in state State_0/None, Cluster 0BMSO+DSSO in state State_0/None, Cluster 0DSSO in state State_0/None, Cluster 0DHSO in state State_0/None, Cluster 0BMSO 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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
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

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling

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	5250000	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	99.79	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

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model