Integrative Structure Validation Report ?

July 22, 2024 - 04:23 PM PDT

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	9A19
PDB-Dev ID	PDBDEV_00000081
Structure Title	Integrative structure of Smc5/6 complex
Structure Authors	Yu Y; Li S; Ser Z; Sanyal T; Choi K; Wan B; Kuang H; Sali A; Kentsis A; Patel DJ; Zhao X

Overall quality ?

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis

Model 1: 7753(99.8 %)

Number of violations
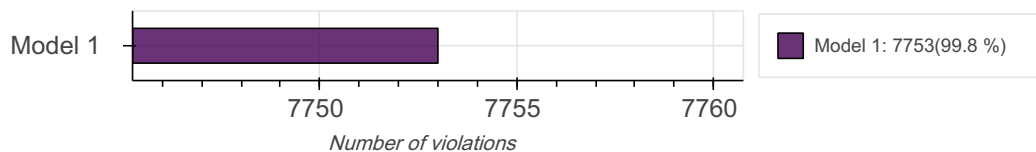
Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 5 subunits in each model. A total of 21 datasets or restraints were used to build this entry. Each model is represented by 35 rigid bodies and 37 flexible or non-rigid units.

Entry composition ?

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	smc5	A	A	1093
1	2	2	smc6	B	B	1114
1	3	3	nse2	C	C	267
1	4	4	nse5	D	D	556
1	5	5	nse6	E	E	464

Datasets used for modeling ?

There are 21 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	6QPW
2	Experimental model	PDB	6ZZ6
3	Comparative model	File	10.5281/zenodo.4685414
4	Comparative model	File	10.5281/zenodo.4685414

ID	Dataset type	Database name	Data access code
5	Comparative model	File	10.5281/zenodo.4685414
6	Experimental model	PDB	3HTK
7	Comparative model	File	10.5281/zenodo.4685414
8	Comparative model	File	10.5281/zenodo.4685414
9	Experimental model	PDB	5MG8
10	Comparative model	File	10.5281/zenodo.4685414
11	Comparative model	File	10.5281/zenodo.4685414
12	Comparative model	File	10.5281/zenodo.4685414
13	Comparative model	File	10.5281/zenodo.4685414
14	Comparative model	File	10.5281/zenodo.4685414
15	Comparative model	File	10.5281/zenodo.4685414
16	Experimental model	PDB	7LTO
17	Experimental model	File	10.5281/zenodo.4685414
18	Mass Spectrometry data	PRIDE	PXD023164
19	Crosslinking-MS data	File	10.5281/zenodo.4685414
20	Crosslinking-MS data	File	10.5281/zenodo.4685414
21	Crosslinking-MS data	File	10.5281/zenodo.4685414

Representation ?

This entry has only one representation and includes 35 rigid bodies and 37 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	42-204, 208-266, 272-302, 304-363, 365-388, 398-459, 485-633, 653-676, 696-714, 719-737, 739-811, 851-880, 885-946, 950-1093	1-41, 205-207, 267-271, 303-303, 364-364, 389-397, 460-484, 634-652, 677-695, 715-718, 738-738, 812-850, 881-884, 947-949

Chain ID	Rigid bodies	Non-rigid segments
B	80-232, 236-294, 298-310, 314-430, 436-501, 506-692, 699-760, 770-882, 897-916, 923-939, 951-984, 988-1114	1-79, 233-235, 295-297, 311-313, 431-435, 502-505, 693-698, 761-769, 883-896, 917-922, 940-950, 985-987
C	5-258	1-4, 259-267
D	22-142, 185-257, 274-441	1-21, 143-184, 258-273, 442-556
E	195-226, 238-379, 387-427, 431-441, 447-464	1-194, 227-237, 380-386, 428-430, 442-446

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	None	20000	False	True
2	1	Replica exchange monte carlo	Sampling	None	100000	False	True

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	develop-31a0ad09b4	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	develop-31a0ad09b4	integrative model building	https://integrativemodeling.org
3	MODELLER	9.25	comparative modeling	https://salilab.org/modeller/
4	SWISS-MODEL	3.0.0	protein homology modeling	https://swissmodel.expasy.org/

Data quality ?

Mass Spectrometry

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

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

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.8	7753.0

Fit of model to data used for modeling ?

Mass Spectrometry

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

IM Structure Validation Report