

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3

Integrative Modeling Validation Version 1.2.1

PDB ID	9A8W
Structure Title	Integrative structure of human SNAPc-DNA
Structure Authors	Shah, S.Z.; Perry, T.N.; Graziadei, A.; Cecatiello, V.; Kaliyappan, T.; Misiaszek, A.D.; Mueller, C.W.; Ramsay, E.P.; Vannini, A.

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

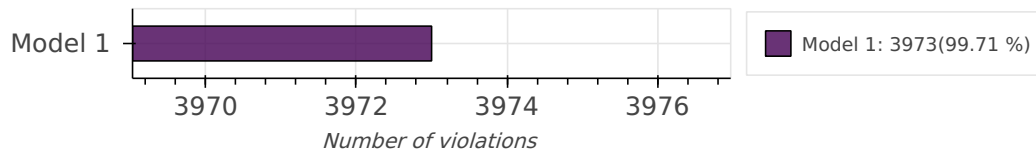
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available [here](#).

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



Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 7 subunits in each model. A total of 8 datasets or restraints were used to build this entry. Each model is represented by 16 rigid bodies and 16 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	snRNA-activating protein complex subunit 2	A	A	334
1	2	2	snRNA-activating protein complex subunit 3	B	B	411
1	3	3	snRNA-activating protein complex subunit 5	C	C	98
1	4	4	snRNA-activating protein complex subunit 1	D	D	368
1	5	5	snRNA-activating protein complex subunit 4	E	E	1519
1	6	6	T strand	F	F	20
1	7	7	NT strand	G	G	20

Datasets used for modeling ?

There are 8 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
5	Crosslinking-MS data	PRIDE	PXD053341
7	3DEM volume	File	10.5281/zenodo.14746890
12	3DEM volume	File	10.5281/zenodo.14746890
8	De Novo model	MODEL ARCHIVE	ma-pgtjz
9	Experimental model	PDB	9FSO
10	Experimental model	PDB	7ZX8
11	Experimental model	PDB	7XUR
6	3DEM volume	EMDB	EMD-50730

Representation ?

This entry has only one representation and includes 16 rigid bodies and 16 flexible units

Chain ID	Rigid bodies	Non-rigid segments
B	27-411	1-26
E	122-163, 182-416, 424-541, 706-799, 806-859, 1304-1434	41-121, 164-181, 417-423, 542-705, 800-805, 860-1303, 1435-1519
C	3-52	1-2, 53-98
D	1-141, 162-234	142-161, 235-368
A	29-87, 97-160, 201-271, 304-334	1-28, 88-96, 161-200, 272-303
F	1-20	-
G	1-20	-

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	320000	False	True

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.20.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.20.0	integrative model building	https://integrativemodeling.org
3	AlphaPulldown	0.30.7	structure prediction	https://github.com/KosinskiLab/AlphaPulldown
4	AlphaFold2	2.3.2	structure prediction	https://github.com/google-deepmind/alphafold

Data quality ?

3DEM volume

Validation for this section is under development.

Crosslinking-MS

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobit 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	99.71	3973.0

Fit of model to data used for modeling ?**3DEM volume**

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.

Acknowledgements

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