Integrative Structure Validation Report July 22, 2024 - 03:57 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	9A05
PDB-Dev ID	PDBDEV_00000041
Structure Title	Integrative structure and function of the yeast exocyst complex
Structure Authors	Ganesan SJ; Feyder MJ; Chemmama IE; Fang F; Rout MP; Chait BT; Shi Y; Munson M; Sali A

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

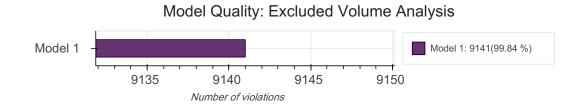
We welcome your comments at pdb-dev@mail.wwpdb.org

A user guide is available at https://pdb-dev.wwpdb.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.



IM Structure Validation Report

Ensemble information @

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 unique models, with 8 subunits in each model. A total of 21 datasets or restraints were used to build this entry. Each model is represented by 43 rigid bodies and 48 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	Sec03	А	А	1336
1	2	2	Sec05	В	В	971
1	3	3	Sec06	С	С	805
1	4	4	Sec08	D	D	1065
1	5	5	Sec10	E	E	871
1	6	6	Sec15	F	F	910
1	7	7	Exo70	G	G	623
1	8	8	Exo84	Н	н	753

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	2PFT

ID	Dataset type	Database name	Data access code
2	Comparative model	File	10.5281/zenodo.3951752
3	Experimental model	PDB	2D2S
4	Comparative model	File	10.5281/zenodo.3951752
5	Experimental model	PDB	2A2F
6	Comparative model	File	10.5281/zenodo.3951752
7	Experimental model	PDB	2FJI
8	Comparative model	File	10.5281/zenodo.3951752
9	Experimental model	PDB	3FHN
10	Comparative model	File	10.5281/zenodo.3951752
11	Experimental model	PDB	5H11
12	Comparative model	File	10.5281/zenodo.3951752
13	Comparative model	File	10.5281/zenodo.3951752
14	Experimental model	PDB	2B1E
15	Experimental model	PDB	1ZC3
16	Comparative model	File	10.5281/zenodo.3951752
17	Experimental model	PDB	2D2S
18	Crosslinking-MS data	File	10.5281/zenodo.3951752
19	Crosslinking-MS data	File	10.5281/zenodo.3951752
20	3DEM volume	EMDB	EMD-21226
21	3DEM volume	File	10.5281/zenodo.3951752

Representation ?

This entry has only one representation and includes 43 rigid bodies and 48 flexible units

4 of 6

Chain ID	Rigid bodies	Non-rigid segments
A	731-884, 924-956, 991-1137, 1157-1223, 1242- 1333	1-730, 885-923, 957-990, 1138-1156, 1224-1241, 1334-1336
В	232-327, 350-371, 457-501, 529-556, 627-658, 686-786, 806-921, 945-957	1-231, 328-349, 372-456, 502-528, 557-626, 659- 685, 787-805, 922-944, 958-971
С	411-805	1-410
D	159-230, 326-361, 393-420, 549-570, 588-610, 631-648, 660-672, 690-698, 745-772, 825-972	1-158, 231-325, 362-392, 421-548, 571-587, 611- 630, 649-659, 673-689, 699-744, 773-824, 973-1065
E	230-280, 319-399, 414-460, 568-624, 639-864	1-229, 281-318, 400-413, 461-567, 625-638, 865- 871
F	474-525, 566-639, 663-685, 703-769	1-473, 526-565, 640-662, 686-702, 770-910
G	67-116, 121-221, 234-295, 301-414, 419-623	1-66, 117-120, 222-233, 296-300, 415-418
Н	344-451, 525-570, 578-647, 650-711, 715-753	1-343, 452-524, 571-577, 648-649, 712-714

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	200000	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.13.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.13.0	integrative model building	https://integrativemodeling.org

ID	Software name	Software version	Software classification	Software location
3	MODELLER	SVN	comparative modeling	https://salilab.org/modeller/

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, 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	99.84	9141.0

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

Development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures, are funded by NSF ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The PDB-Dev team and members of Sali labcontributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded byRCSB PDB (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from RCSB PDB, Dr. Jill Trewhella, Dr. Dina Schneidman, and members of the SASBDB repository are acknowledged for their advice and support in implementing SAS validation methods.

Members of the wwPDB Integrative/Hybrid Methods Task Force provided recommendations and community support for the project.