Integrative Structure Validation Report

February 18, 2025 - 08:29 AM PST

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

Integrative Modeling Validation Version 2.0
Python-IHM Version 1.8

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
Deposited on	2020-02-04

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

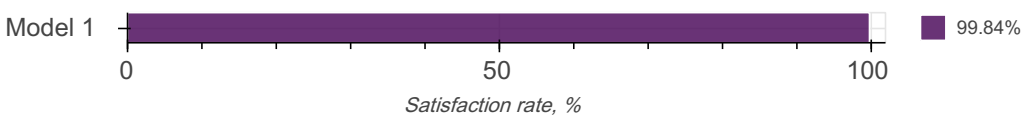
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

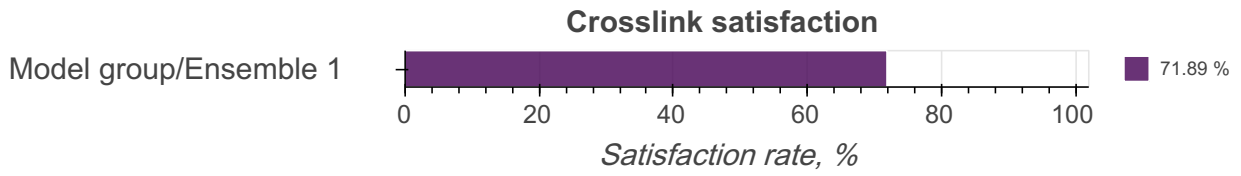
List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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 model(s). A total of 21 datasets were used to build this entry.

Representation

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Sec03	A	1336	731-884, 924-956, 991-1137, 1157-1223, 1242-1333	1-730, 885-923, 957-990, 1138-1156, 1224-1241, 1334-1336	100.00 / 36.90	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		2	Sec05	B	971	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	100.00 / 46.65	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		3	Sec06	C	805	411-805	1-410	100.00 / 49.07	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	Sec08	D	1065	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	100.00 / 37.28	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		5	Sec10	E	871	230-280, 319-399, 414-460, 568-624, 639-864	1-229, 281-318, 400-413, 461-567, 625-638, 865-871	100.00 / 53.04	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		6	Sec15	F	910	474-525, 566-639, 663-685, 703-769	1-473, 526-565, 640-662, 686-702, 770-910	100.00 / 23.74	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		7	Exo70	G	623	67-116, 121-221, 234-295, 301-414, 419-623	1-66, 117-120, 222-233, 296-300, 415-418	100.00 / 85.39	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		8	Exo84	H	753	344-451, 525-570, 578-647, 650-711, 715-753	1-343, 452-524, 571-577, 648-649, 712-714	100.00 / 43.16	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead

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
2	Comparative model	Zenodo	10.5281/zenodo.3951752

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

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	Sampling	Replica exchange monte carlo	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
3	MODELLER	SVN	comparative modeling	https://salilab.org/modeller/

Data quality

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully compliant dataset in the PRIDE Crosslinking database. Correspondence between crosslinking-MS and entry entities is established using pyHMMER. Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the PRIDE Crosslinking database.

3DEM volume

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. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	5717271	9141	99.84

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". Restraint group represents a set of crosslinking restraints applied collectively in the modeling.

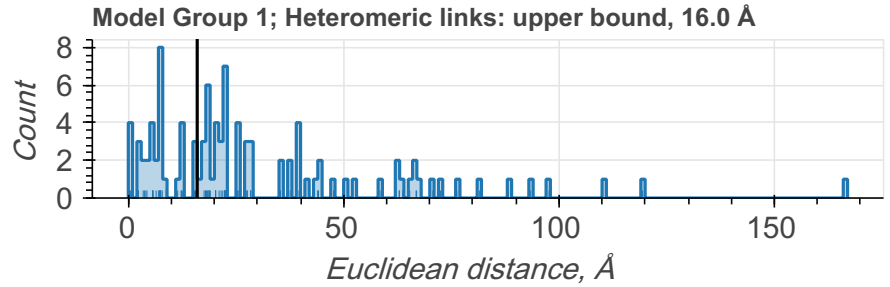
There are 434 crosslinking restraints combined in 434 restraint groups.

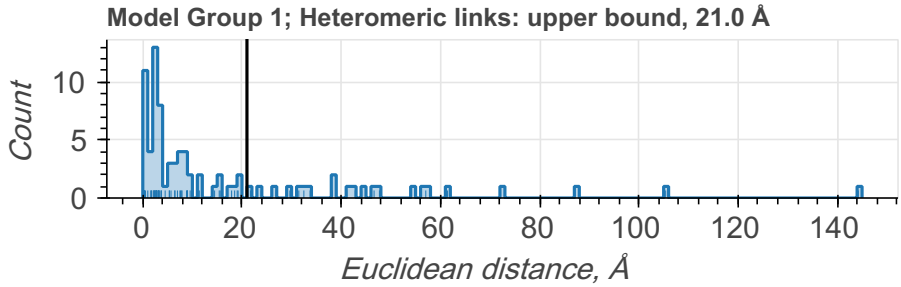
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	21.0	207
DSS	LYS	CA	LYS	CA	upper bound	21.0	43

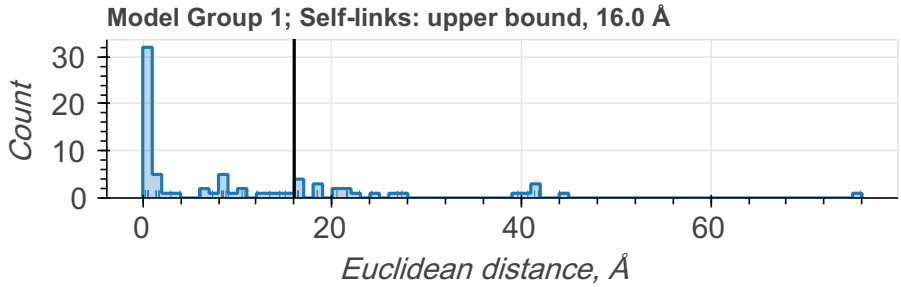
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	coarse-grained	VAL	coarse-grained	upper bound	21.0	2
DSS	LYS	coarse-grained	PRO	coarse-grained	upper bound	21.0	4
EDC	GLU	coarse-grained	LYS	coarse-grained	upper bound	16.0	105
EDC	ASP	coarse-grained	LYS	coarse-grained	upper bound	16.0	54
EDC	GLU	CA	LYS	CA	upper bound	16.0	15
EDC	ASP	CA	LYS	CA	upper bound	16.0	4

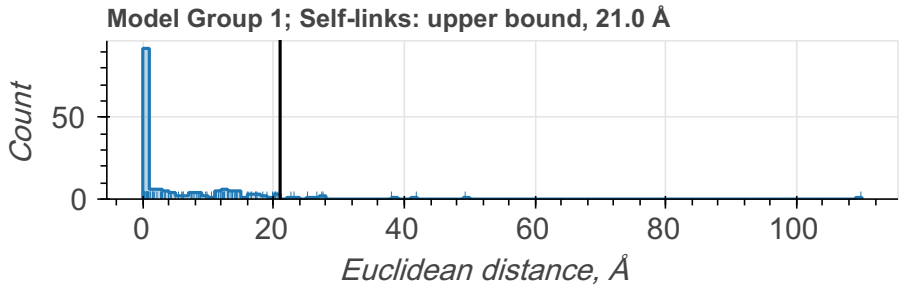
Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.









Satisfaction of restraints

Satisfaction of restraints is calculated on a restraint group (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=434)
1	1	1	1/9669	All	71.89	28.11	434
				Heteromeric links/ Intermolecular	51.61	48.39	186
				Self-links/ Intramolecular	87.10	12.90	248

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgments

The 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 awards to the PDB-IHM team (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the RCSB PDB (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the Sali lab contributed model validation metrics and software packages.

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