Integrative Structure Validation Report

July 22, 2024 - 03:46 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	8ZZL
PDB-Dev ID	PDBDEV_00000021
Structure Title	Structure of complement C3(H2O) revealed by quantitative cross-linking/mass spectrometry and modeling
Structure Authors	Chen ZA; Pellarin R; Fischer L; Sali A; Nilges M; Barlow PN; Rappsilber J

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

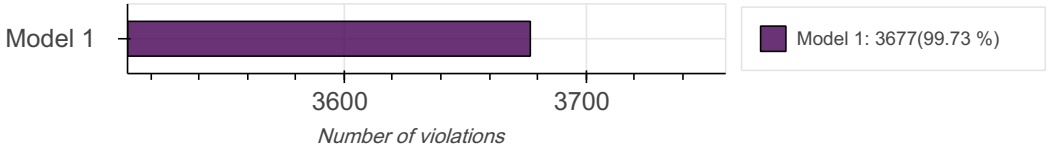
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

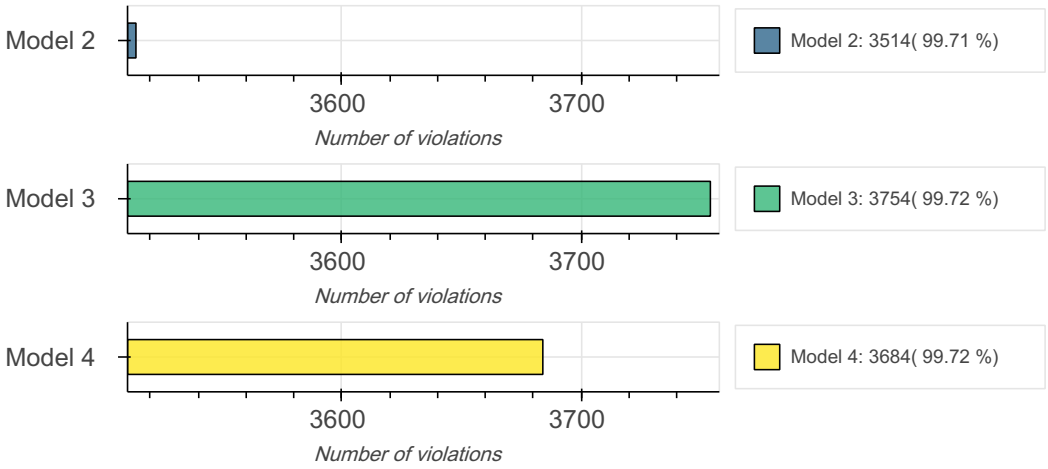
List of references used to build this report is available here.

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.

Model Quality: Excluded Volume Analysis





Ensemble information

This entry consists of 4 distinct ensemble(s).

Summary

This entry consists of 4 unique models, with 2 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 13 rigid bodies and 12 flexible or non-rigid units.

Entry composition

There are 4 unique types of models in this entry.These models are titled C3 cluster 1/Best scoring model, C3b cluster 1/Best scoring model, iC3 cluster 1/Best scoring model, iC3 cluster 2/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	beta	A	A	645
1	2	2	alpha	B	B	992
2	1	1	beta	A	A	645
2	2	2	alpha	B	B	992
3	1	1	beta	A	A	645
3	2	2	alpha	B	B	992
4	1	1	beta	A	A	645

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
4	2	2	alpha	B	B	992

Datasets used for modeling

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	2A73
2	Experimental model	PDB	2I07
3	Mass Spectrometry data	PRIDE	PXD003486
4	Crosslinking-MS data	File	10.5281/zenodo.1285940

Representation

This entry has only one representation and includes 13 rigid bodies and 12 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-73, 80-289, 292-643	74-79, 290-291, 644-645
B	2-70, 80-96, 97-155, 158-261, 264-312, 315-457, 464-618, 621-680, 683-824, 827-992	1-1, 71-79, 156-157, 262-263, 313-314, 458-463, 619-620, 681-682, 825-826

Methodology and software

This entry is a result of 3 distinct protocol(s).

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

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	True	True
1	2	Replica exchange monte carlo	Sampling	None	200000	True	True
1	3	Replica exchange monte carlo	Sampling	None	200000	True	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org
2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling.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

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.73	3677.0
2	99.71	3514.0
3	99.72	3754.0
4	99.72	3684.0

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.

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.