

Integrative Structure Validation Report ?

February 18, 2025 - 08:28 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	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
Deposited on	2018-06-06

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

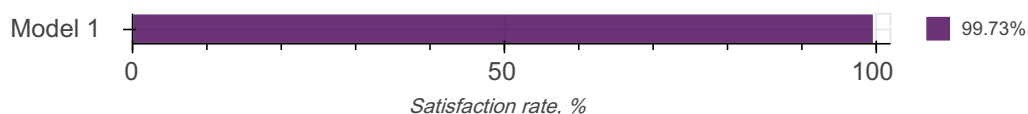
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

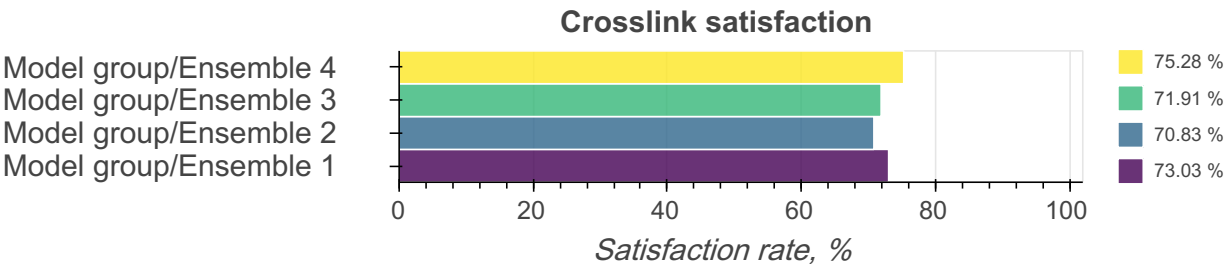
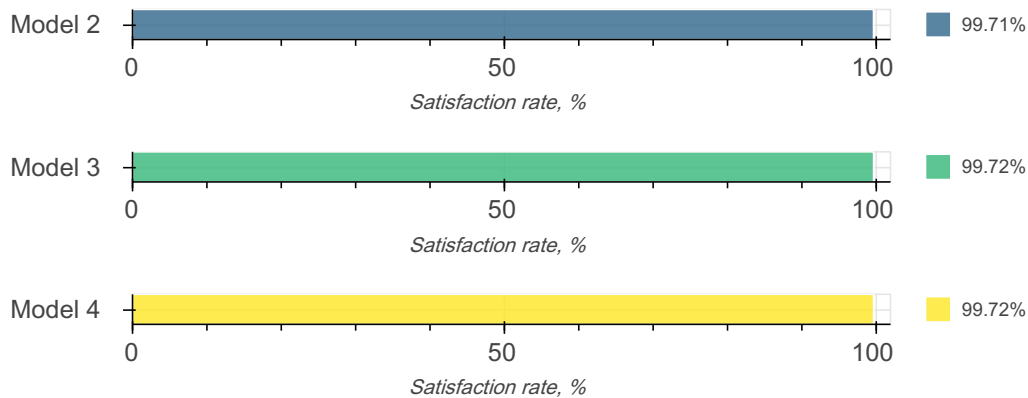
List of references used to build this report is available [here](#).

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 4 distinct ensemble(s).

Summary ?

This entry consists of 4 model(s). A total of 4 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	1-4	1	beta	A	645	1-73, 80-289, 292-643	74-79, 290-291, 644-645	100.00 / 98.45	Coarse-grained: 1 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
		2	alpha	B	992	2-70, 80-96, 97-155, 158-261, 264-312, 315-457, 464-618, 621-680, 683-824, 827-992	1, 71-79, 156-157, 262-263, 313-314, 458-463, 619-620, 681-682, 825-826	100.00 / 97.18	Coarse-grained: 1 residue(s) per bead

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	Zenodo	10.5281/zenodo.1285940

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

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.

Mass Spectrometry

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-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	1339066	3677	99.73
2	1216020	3514	99.71
3	1339066	3754	99.72
4	1339066	3684	99.72

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

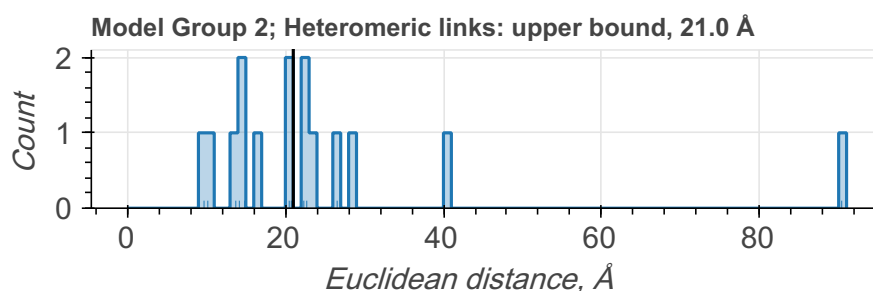
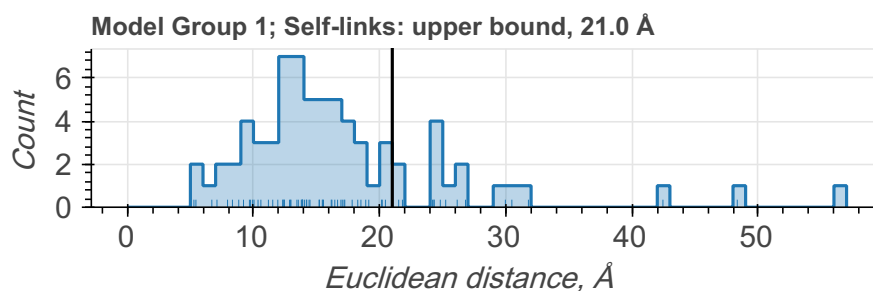
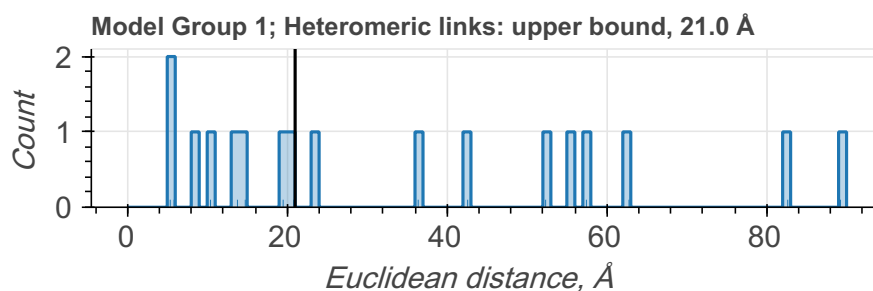
Restraint types are summarized in the table below. Restraints assigned "[by-residue](#)" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "[coarse-grained](#)". [Restraint group](#) represents a set of crosslinking restraints applied collectively in the modeling.

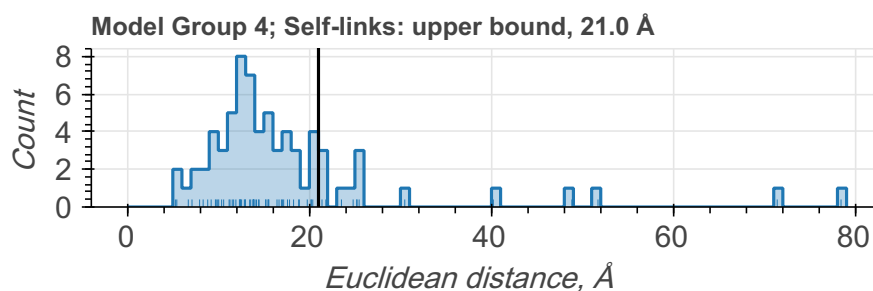
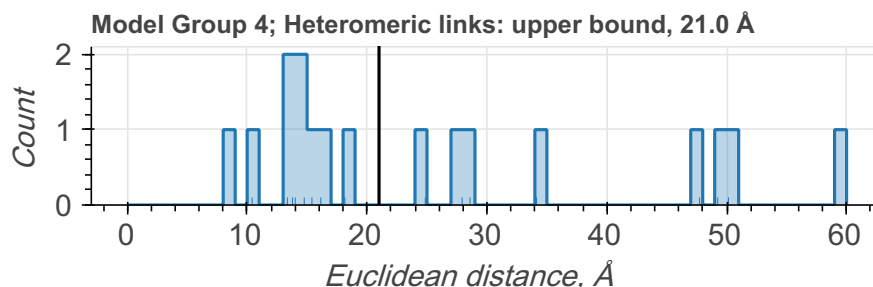
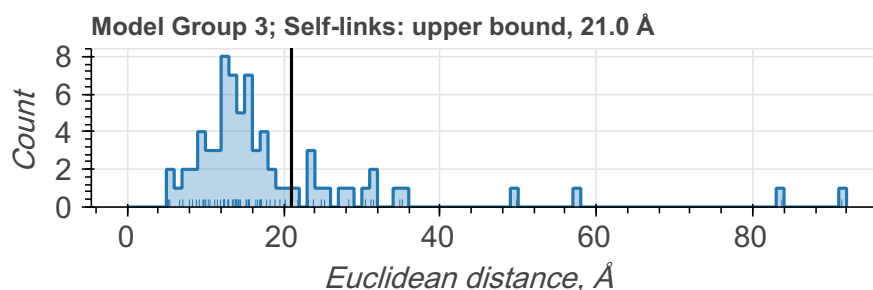
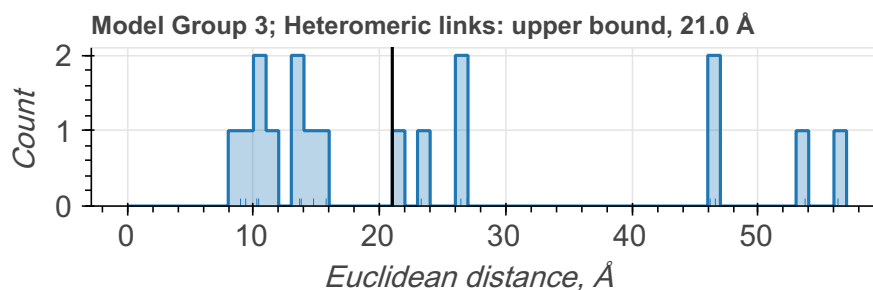
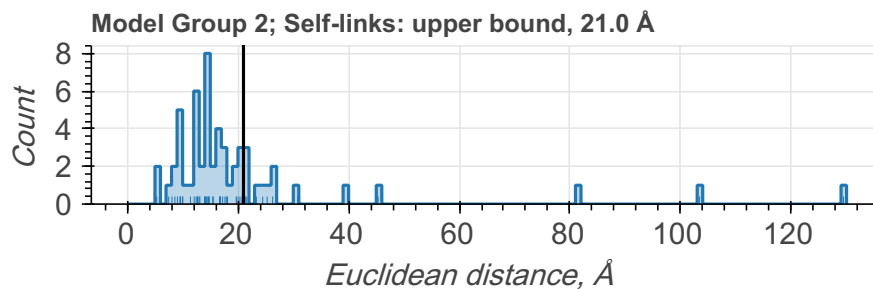
There are 115 crosslinking restraints combined in 115 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	LYS	CA	upper bound	21.0	78
BS3	LYS	CA	SER	CA	upper bound	21.0	21
BS3	SER	CA	SER	CA	upper bound	21.0	4
BS3	LYS	CA	TYR	CA	upper bound	21.0	5
BS3	SER	CA	TYR	CA	upper bound	21.0	3
BS3	LYS	CA	THR	CA	upper bound	21.0	3
BS3	THR	CA	THR	CA	upper bound	21.0	1

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

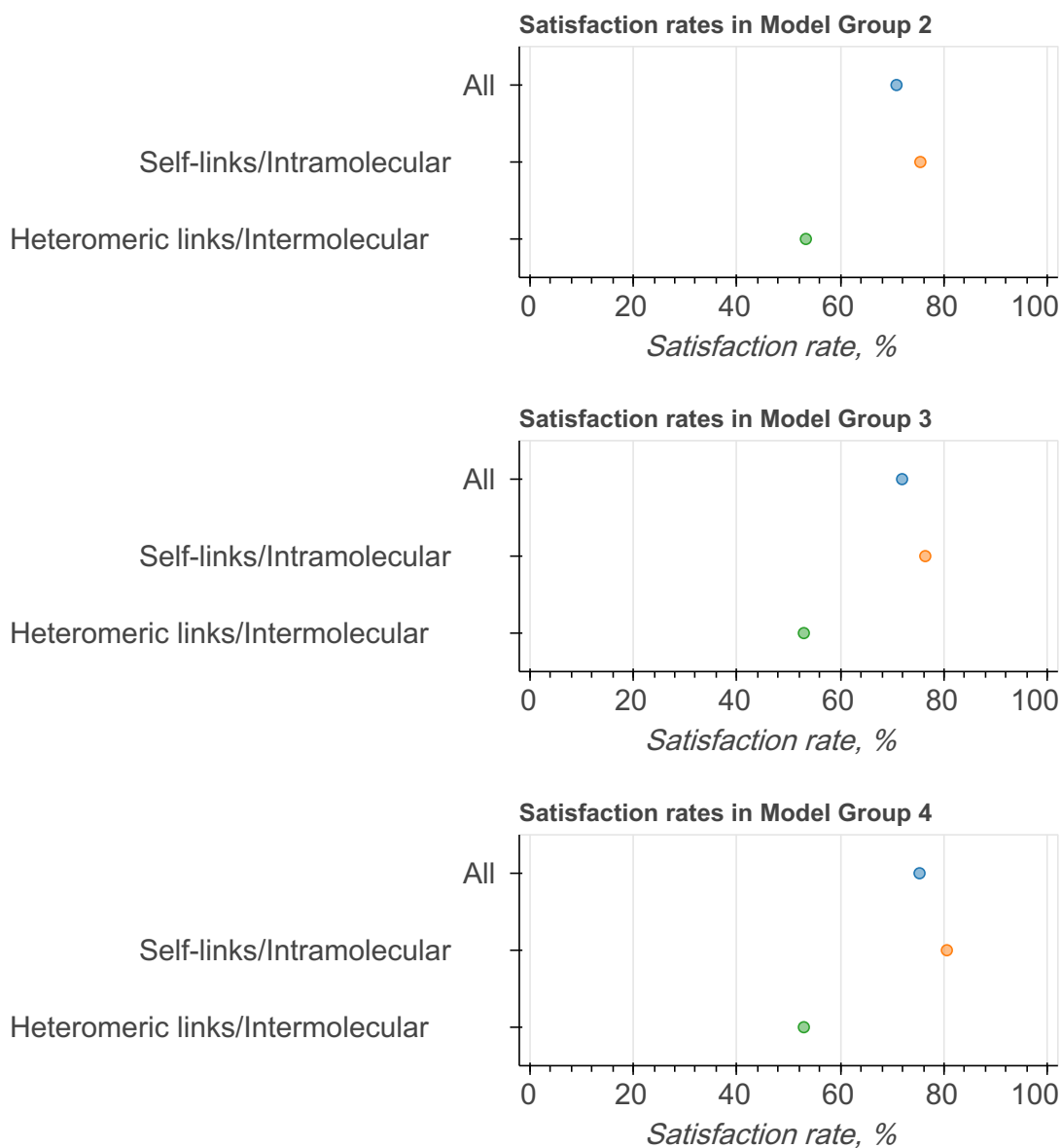
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=115)
1	1	1	1/200	All	73.03	26.97	89
				Self-links/ Intramolecular	79.17	20.83	72
				Heteromeric links/ Intermolecular	47.06	52.94	17
1	2	2	1/200	All	70.83	29.17	72
				Self-links/ Intramolecular	75.44	24.56	57
				Heteromeric links/ Intermolecular	53.33	46.67	15
1	3	3	1/89	All	71.91	28.09	89
				Self-links/ Intramolecular	76.39	23.61	72
				Heteromeric links/ Intermolecular	52.94	47.06	17
1	3	4	1/111	All	75.28	24.72	89
				Self-links/ Intramolecular	80.56	19.44	72
				Heteromeric links/ Intermolecular	52.94	47.06	17

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.





Mass Spectrometry

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](#)

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