

# Integrative Structure Validation Report ?

March 27, 2025 - 10:01 AM PDT

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

*Integrative Modeling Validation Version 2.0*

*Python-IHM Version 1.8*

PDB ID	9A0E
PDB-Dev ID	PDBDEV_00000050
Structure Title	Structural basis of CD4 downregulation by HIV-1 Nef
Structure Authors	Kwon Y; Kaake RM; Echeverria I; Suarez M; Karimian Shamsabadi M; Stoneham C; Ramirez PW; Kress J; Singh R; Sali A; Krogan N; Guatelli J; Jia X
Deposited on	2020-05-19

*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](mailto:helpdesk@pdb-ihm.org)*

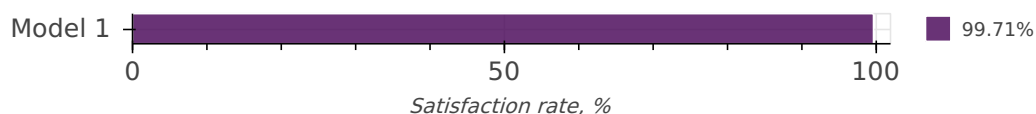
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

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

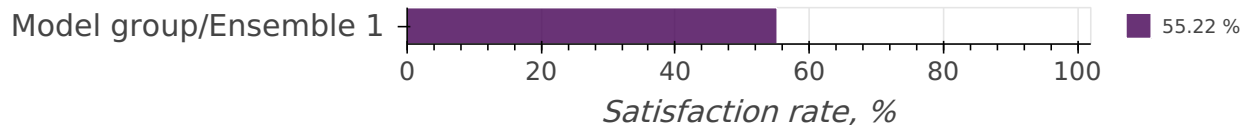
## Overall quality ?

*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



## Crosslink satisfaction



## Ensemble information ?

*This entry consists of 1 distinct ensemble(s).*

## Summary ?

*This entry consists of 1 model(s). A total of 5 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	Nef	A	202	13-182	1-12, 183-202	100.00 / 84.16	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
		2	CD4mut	B	26	12-25	1-11, 26	100.00 / 53.85	Coarse-grained: 1 residue(s) per bead
		3	AP2alpha2	C	627	9-619	1-8, 620-627	100.00 / 97.45	Coarse-grained: 1 residue(s) per bead
		4	AP2mu2	D	135	1-124	125-135	100.00 / 91.85	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
		5	AP2sigma	E	142	1-142	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		6	AP2beta2	F	591	15-23, 29-43, 49-61, 64-78, 81-86, 91-583	1-14, 24-28, 44-48, 62-63, 79-80, 87-90, 584-591	100.00 / 93.23	Coarse-grained: 1 residue(s) per bead

### Datasets used for modeling ?

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.3836213">10.5281/zenodo.3836213</a>
2	Experimental model	PDB	<a href="https://www.rcsb.org/structure/2VGL">2VGL</a>
3	Comparative model	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.3836213">10.5281/zenodo.3836213</a>
4	Mass Spectrometry data	PRIDE	<a href="https://www.ebi.ac.uk/pride/archive/entry/PXD019338">PXD019338</a>
5	Crosslinking-MS data	Zenodo	<a href="https://zenodo.org/record/10.5281/zenodo.3836213">10.5281/zenodo.3836213</a>

### 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	2007800	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
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ID	Software name	Software version	Software classification	Software location
1	<a href="#">IMP PMI module</a>	develop-29bf2b61d4	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
2	<a href="#">Integrative Modeling Platform (IMP)</a>	develop-29bf2b61d4	integrative model building	<a href="https://integrativemodeling.org">https://integrativemodeling.org</a>
3	<a href="#">MODELLER</a>	9.22	comparative modeling	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>

## 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	1440753	4163	99.71

## Fit of model to data used for modeling ?

### Fit of model(s) to crosslinking-MS data

## Restraint types

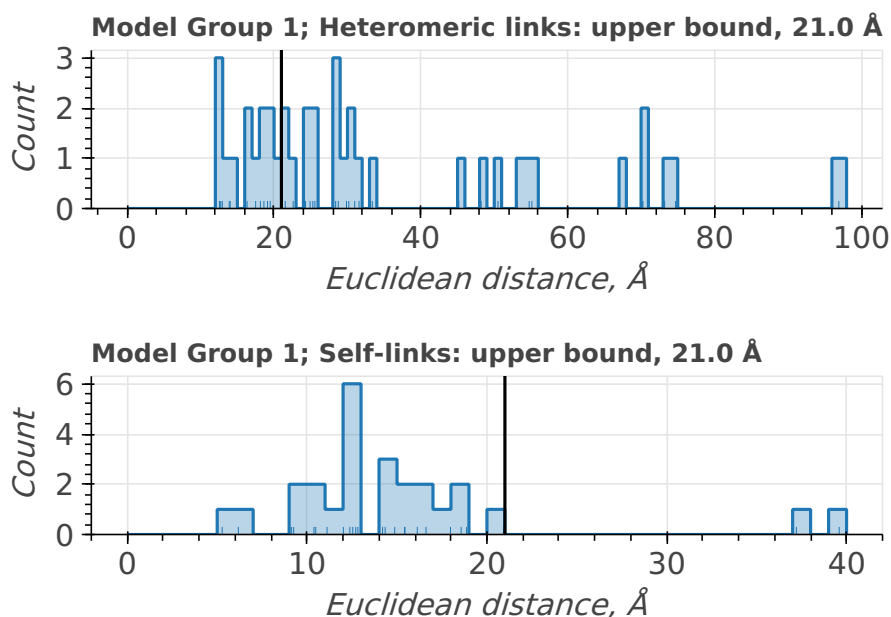
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 90 crosslinking restraints combined in 90 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	21.0	87
DSSO	ALA	coarse-grained	LYS	coarse-grained	upper bound	21.0	2
DSSO	ARG	CA	LYS	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.



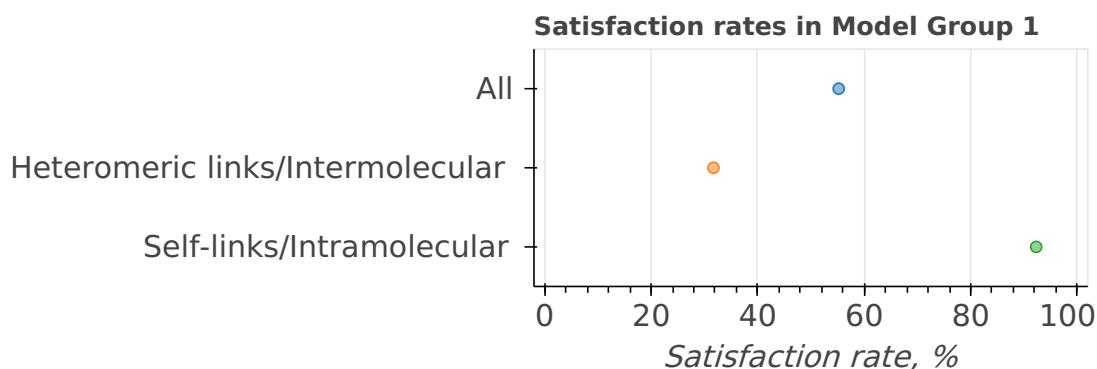
## Satisfaction of restraints

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=90)
1	1	1	1/9999	All	55.22	44.78	67
				Heteromeric links/ Intermolecular	31.71	68.29	41
				Self-links/ Intramolecular	92.31	7.69	26

#### 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](#) (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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*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*