

**Summary of integrative structure determination of Structural basis of
CD4 downregulation by HIV-1 Nef (PDB ID: 9A0E, PDB-Dev ID:
PDBDEV_00000050)**

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Nef: chain(s) A (202 residues) - CD4mut: chain(s) B (26 residues) - AP2alpha2: chain(s) C (627 residues) - AP2mu2: chain(s) D (135 residues) - AP2sigma: chain(s) E (142 residues) - AP2beta2: chain(s) F (591 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, Zenodo: 10.5281/zenodo.3836213 - Experimental model, PDB: 2VGL - Comparative model, Zenodo: 10.5281/zenodo.3836213 - Mass Spectrometry data, PRIDE: PXD019338 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3836213
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
Number of <i>rigid</i> and <i>flexible</i> segments	11, 14
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 90 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	9999
Number of deposited models	1
Model precision (uncertainty of models)	8.30, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.71%
Fit to data used for modeling	Satisfaction of crosslinks: 55.22%

<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	2007800
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version develop-29bf2b61d4) - Integrative Modeling Platform (IMP) (version develop-29bf2b61d4) - MODELLER (version 9.22)