

**Summary of integrative structure determination of Structural basis of CD4 downregulation by HIV-1 Nef (PDB ID: 9A0E, PDB-Dev ID: PDBDEV\_0000050)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- AP2beta2: Chain F (591 residues)</li> <li>- Nef: Chain A (242 residues)</li> <li>- CD4mut: Chain B (419 residues)</li> <li>- AP2mu2: Chain D (135 residues)</li> <li>- AP2alpha2: Chain C (627 residues)</li> <li>- AP2sigma: Chain E (142 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: Not available</li> <li>- Experimental model, PDB ID: 2VGL</li> <li>- Comparative model, template PDB ID: Not available</li> <li>- Mass Spectrometry data, PRIDE: PXD019338</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSSO, 90 cross-links</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Coarse-grained: 1, 2, 3, 4, 5, 8, 11, 14 residue(s) per bead
<a href="#">Number of rigid bodies, flexible units</a>	11, 14
<a href="#">Rigid bodies</a>	<ul style="list-style-type: none"> <li>- A: 33-202</li> <li>- B: 405-418</li> <li>- C: 9-619</li> <li>- D: 1-124</li> <li>- E: 1-142</li> <li>- F: 15-23, 29-43, 49-61, 64-78, 81-86, 91-583</li> </ul>
<a href="#">Flexible units</a>	<ul style="list-style-type: none"> <li>- A: 21-32, 203-222</li> <li>- B: 394-404, 419-419</li> <li>- C: 1-8, 620-627</li> <li>- D: 125-135</li> <li>- E: -</li> <li>- F: 1-14, 24-28, 44-48, 62-63, 79-80, 87-90, 584-591</li> </ul>
<a href="#">Structural coverage (rigid bodies)</a>	94%
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: DSSO, 90 cross-links
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	9999

<a href="#"><i>Number of deposited models</i></a>	1
<a href="#"><i>Model precision (uncertainty of models)</i></a>	8.3, Å
<a href="#"><i>Data quality</i></a>	Data quality has not been assessed
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	Satisfaction: 99.71-99.71%
<a href="#"><i>Fit to data used for modeling</i></a>	Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<b>1. Method</b>	Sampling
<a href="#"><i>Name</i></a>	Replica exchange monte carlo
<a href="#"><i>Number of computed models</i></a>	2007800
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">IMP PMI module</a> (version develop-29bf2b61d4)</li> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version develop-29bf2b61d4)</li> <li>- <a href="#">MODELLER</a> (version 9.22)</li> </ul>