

**Summary of integrative structure determination of Photoinduced intermediate I of bacteriorhodopsin at ~400 femtosecond with an expanded retinal binding pocket (PDB ID: 9A21, PDB-Dev ID: PDBDEV\_00000138)**

<b>1. Model Composition</b>	
<a href="#"><u>Entry composition</u></a>	<ul style="list-style-type: none"> <li>- RETINAL: Chain B (Not available residues)</li> <li>- water: Chain C (8 residues)</li> <li>- BACTERIORHODOPSIN: Chain A (248 residues)</li> </ul>
<a href="#"><u>Datasets used for modeling</u></a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 6g7h</li> <li>- Other, PDB: 6g7h</li> <li>- Other, PDB: 6g7i</li> <li>- Other, PDB: 6g7j</li> <li>- Other, PDB: 6g7k</li> <li>- Other, PDB: 6ga2</li> <li>- Other, PDB: 6ga4</li> <li>- Other, PDB: 6ga5</li> <li>- Other, PDB: 6ga6</li> <li>- Other, PDB: 6ga7</li> <li>- Other, PDB: 6ga8</li> <li>- Other, PDB: 6ga9</li> <li>- Other, PDB: 6gaa</li> <li>- Other, PDB: 6gab</li> <li>- Other, PDB: 6gac</li> <li>- Other, PDB: 6gad</li> <li>- Other, PDB: 6gae</li> <li>- Other, PDB: 6gaf</li> <li>- Other, PDB: 6gag</li> <li>- Other, PDB: 6gah</li> <li>- Other, PDB: 6gai</li> </ul>
<b>2. Representation</b>	
<a href="#"><u>Resolution</u></a>	Atomic
<a href="#"><u>Number of rigid bodies, flexible units</u></a>	0, 3
<a href="#"><u>Flexible units</u></a>	<ul style="list-style-type: none"> <li>- A: 1-248</li> <li>- B: None-None</li> <li>- C: 1-8</li> </ul>
<a href="#"><u>Structural coverage (rigid bodies)</u></a>	100%
<b>3. Restraints</b>	
<a href="#"><u>Physical principles</u></a>	Information about physical principles was not provided
<a href="#"><u>Experimental data</u></a>	
<b>4. Validation</b>	
<a href="#"><u>Number of ensembles</u></a>	0
<a href="#"><u>Number of models in ensembles</u></a>	Not applicable

<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Model precision can not be calculated with one structure
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 4.68, Number of Ramachandran outliers = 1, Number of sidechain outliers = 12
<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<u>1. Method</u>	Singular value decomposition analysis of difference Fourier maps
<u>Name</u>	Singular value decomposition
<u>Number of computed models</u>	1
<u>Software</u>	- PHENIX (version (1.13_2998: ???)) - dynamiX (version Not available)