

Summary of integrative structure determination of Photoinduced intermediate J' of bacteriorhodopsin from 0.5 to 2 picosecond immediately after photoisomerization (PDB ID: 9A22, PDB-Dev ID: PDBDEV_00000139)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - RETINAL: Chain B (Not available residues) - BACTERIORHODOPSIN: Chain A (248 residues) - water: Chain C (6 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 6g7h - Other, PDB: 6g7h - Other, PDB: 6g7i - Other, PDB: 6g7j - Other, PDB: 6g7k - Other, PDB: 6ga2 - Other, PDB: 6ga4 - Other, PDB: 6ga5 - Other, PDB: 6ga6 - Other, PDB: 6ga7 - Other, PDB: 6ga8 - Other, PDB: 6ga9 - Other, PDB: 6gaa - Other, PDB: 6gab - Other, PDB: 6gac - Other, PDB: 6gad - Other, PDB: 6gae - Other, PDB: 6gaf - Other, PDB: 6gag - Other, PDB: 6gah - Other, PDB: 6gai
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	0, 3
<u>Flexible units</u>	<ul style="list-style-type: none"> - A: 1-248 - B: None-None - C: 1-6
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	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 = 21
<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
5. Methodology and Software	
<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)