

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)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - BACTERIORHODOPSIN: chain(s) A (248 residues) - RETINAL: chain(s) B [A] - water: chain(s) C [A]
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 6g7h - X-ray diffraction data, PDB: 6g7h - X-ray diffraction data, PDB: 6g7i - X-ray diffraction data, PDB: 6g7j - X-ray diffraction data, PDB: 6g7k - X-ray diffraction data, PDB: 6ga2 - X-ray diffraction data, PDB: 6ga4 - X-ray diffraction data, PDB: 6ga5 - X-ray diffraction data, PDB: 6ga6 - X-ray diffraction data, PDB: 6ga7 - X-ray diffraction data, PDB: 6ga8 - X-ray diffraction data, PDB: 6ga9 - X-ray diffraction data, PDB: 6gaa - X-ray diffraction data, PDB: 6gab - X-ray diffraction data, PDB: 6gac - X-ray diffraction data, PDB: 6gad - X-ray diffraction data, PDB: 6gae - X-ray diffraction data, PDB: 6gaf - X-ray diffraction data, PDB: 6gag - X-ray diffraction data, PDB: 6gah - X-ray diffraction data, PDB: 6gai
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1

<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 4.68 - Ramachandran outliers: 1 - Sidechain outliers: 12
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<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>	Singular value decomposition analysis of difference Fourier maps
<i>Method</i>	Singular value decomposition
<i>Number of computed models</i>	1
<i>Software</i>	<ul style="list-style-type: none"> - PHENIX (version (1.13_2998: ???)) - dynamix (version Not available)