

Summary of integrative structure determination of Photoinduced intermediate J of bacteriorhodopsin from 1 to 30 picosecond with a contracted retinal binding pocket (PDB ID: 9A23, PDB-Dev ID: PDBDEV_00000140)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - BACTERIORHODOPSIN: Chain A (248 residues) - water: Chain C (5 residues) - RETINAL: Chain B (Not available residues)
Datasets used for modeling	<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	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 3
Flexible units	<ul style="list-style-type: none"> - A: 1-248 - B: None-None - C: 1-5
Structural coverage (rigid bodies)	100%
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

<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	Model-1: Clashscore = 6.89, Number of Ramachandran outliers = 1, Number of sidechain outliers = 17
<i>Model quality: assessment of excluded volume</i>	Not applicable
<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>Method</i>	Singular value decomposition analysis of difference Fourier maps
<i>Name</i>	Singular value decomposition
<i>Number of computed models</i>	1
<i>Software</i>	- PHENIX (version (1.13_2998: ???)) - dynamiX (version Not available)