

Summary of integrative structure determination of Photoinduced intermediate M2 of bacteriorhodopsin from 0.5 to 5 millisecond (PDB ID: 9A29, PDB-Dev ID: PDBDEV_00000147)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - RETINAL: Chain B (Not available residues) - water: Chain C (6 residues) - BACTERIORHODOPSIN: Chain A (230 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 6g7h - Other, PDB: 5b6v - Other, PDB: 5b6w - Other, PDB: 5b6x - Other, PDB: 5b6y - Other, PDB: 5b6z - Other, PDB: 5h2h - Other, PDB: 5h2i - Other, PDB: 5h2j - Other, PDB: 5h2k - Other, PDB: 5h2l - Other, PDB: 5h2m - Other, PDB: 5h2n - Other, PDB: 5h2o - Other, PDB: 5h2p - Other, PDB: 6g7h - Other, PDB: 6g7l - Other, PDB: 6ga1 - Other, PDB: 6ga2 - Other, PDB: 6ga3 - Other, PDB: 6rmk - Other, PDB: 6rnj - Other, PDB: 6rph - Other, PDB: 6rqo - Other, PDB: 6rqp
2. Representation	
Resolution	Atomic
Number of <i>rigid bodies</i>, <i>flexible units</i>	0, 3
Flexible units	<ul style="list-style-type: none"> - A: 5-234 - B: None-None - C: 1-6
Structural coverage (<i>rigid bodies</i>)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	
4. Validation	

<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	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 = 7.16, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21
<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)