

Summary of integrative structure determination of Photoinduced intermediate M1 of bacteriorhodopsin from 10 to 1000 microsecond with a flooded cytoplasmic half channel (PDB ID: 9A28, PDB-Dev ID: PDBDEV_00000146)

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: 5b6v - X-ray diffraction data, PDB: 5b6w - X-ray diffraction data, PDB: 5b6x - X-ray diffraction data, PDB: 5b6y - X-ray diffraction data, PDB: 5b6z - X-ray diffraction data, PDB: 5h2h - X-ray diffraction data, PDB: 5h2i - X-ray diffraction data, PDB: 5h2j - X-ray diffraction data, PDB: 5h2k - X-ray diffraction data, PDB: 5h2l - X-ray diffraction data, PDB: 5h2m - X-ray diffraction data, PDB: 5h2n - X-ray diffraction data, PDB: 5h2o - X-ray diffraction data, PDB: 5h2p - X-ray diffraction data, PDB: 6g7h - X-ray diffraction data, PDB: 6g7l - X-ray diffraction data, PDB: 6ga1 - X-ray diffraction data, PDB: 6ga2 - X-ray diffraction data, PDB: 6ga3 - X-ray diffraction data, PDB: 6rmk - X-ray diffraction data, PDB: 6rnj - X-ray diffraction data, PDB: 6rph - X-ray diffraction data, PDB: 6rqo - X-ray diffraction data, PDB: 6rqp
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible 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

<i>Number of deposited models</i>	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: 9.64 - Ramachandran outliers: 0 - Sidechain outliers: 25
<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)