

Summary of integrative structure determination of Photoinduced intermediate L of bacteriorhodopsin from 1 to 100 microsecond with a flattened 13-cis retinal (PDB ID: 9A27, PDB-Dev ID: PDBDEV_00000145)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - BACTERIORHODOPSIN: Chain A (230 residues) - water: Chain C (4 residues) - RETINAL: Chain B (Not available residues)
<u>Datasets used for modeling</u>	<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	
<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: 5-234 - B: None-None - C: 1-4
<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 = 7.99, Number of Ramachandran outliers = 0, Number of sidechain outliers = 23
<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	
1. <u>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)