

Summary of integrative structure determination of Photoinduced intermediate K of bacteriorhodopsin from 3 picosecond to 2 microsecond with a lifetime of more than five decades (PDB ID: 9A26, PDB-Dev ID: PDBDEV_00000144)

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| 1. Model Composition | |
| Entry composition | <ul style="list-style-type: none"> - water: Chain C (8 residues) - BACTERIORHODOPSIN: Chain A (230 residues) - RETINAL: Chain B (Not available 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: 1-8 |
| Structural coverage (<i>rigid bodies</i>) | 100% |
| 3. Restraints | |
| Physical principles | Information about physical principles was not provided |
| Experimental data | |
| 4. Validation | |

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| <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 = 6.89, Number of Ramachandran outliers = 1, Number of sidechain outliers = 11 |
| <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) |