

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"> - 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: 7.16 - Ramachandran outliers: 1 - Sidechain outliers: 21 |
| <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) |